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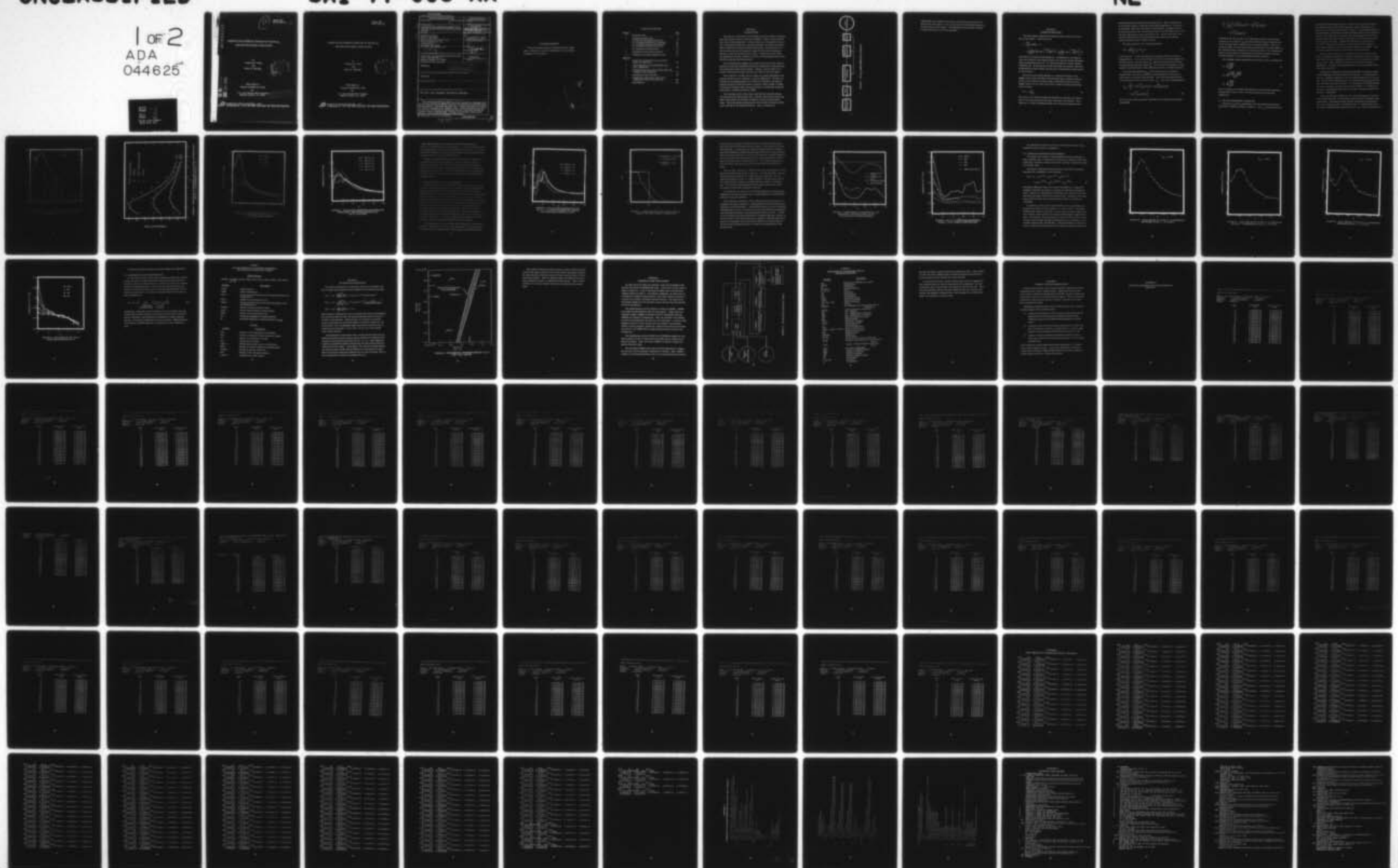

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by
Frederick G. Smith
and
Robert E. Meredith

Final Report on
Contract DAAK40-76-C-0754
for
U. S. Army Missile R&D Command
Redstone Arsenal, AL 35809

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The linewidth and Einstein coefficient values required for modeling the HCl non-reacting mixing laser (NRML) have been reviewed and new linewidth calculations prepared. The results have been fit to a simple functional form suitable for inclusion in detailed laser modeling codes. Further development was also carried out of an efficient non-equilibrium chemistry subroutine suitable for inclusion in laser modeling codes. Listings of the detailed results and the chemistry code are given in appendices of the report.

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SECTION 1
INTRODUCTION

The program reported here was initiated to improve computer modeling of the $HCl-H_2$ non-reacting mixing laser (NRML). Figure 1 illustrates the basic laser modeling approach. In the present case, the equilibrium chemistry modeling represents the combustion processes occuring in the plenum where a solid fuel is burned to produce HCl and H_2. Fluid dynamics routines describe the flow of the gases through the throat and the expansion through a nozzle into the laser cavity region. Downstream of the nozzle, non-equilibrium chemistry models represent the HCl pumping reactions and the HCl and H_2 deactivation processes.

The resulting specie populations are then used with the basic radiative properties (molecular linewidths and Einstein coefficients) to determine the incremental gain profile of the medium. Finally, a cavity model is employed to determine the power and spectral content of the laser output.

The complexities of laser device models vary greatly depending on the purpose and the accuracy required in a specific application. We have concentrated on developing general non-equilibrium chemistry and radiative property programs which can be basic modules in either simple or sophisticated laser modeling codes; and the generation or compilation of specific input data for modeling the $HCl-H_2$ NRML.

The following section of this report describes the linewidth calculations performed for this program and a computer subroutine incorporating these results which may be easily included in most laser performance codes. The third section summarizes the current status of Einstein coefficient modeling for HCl lasing transitions. Next, we discuss the

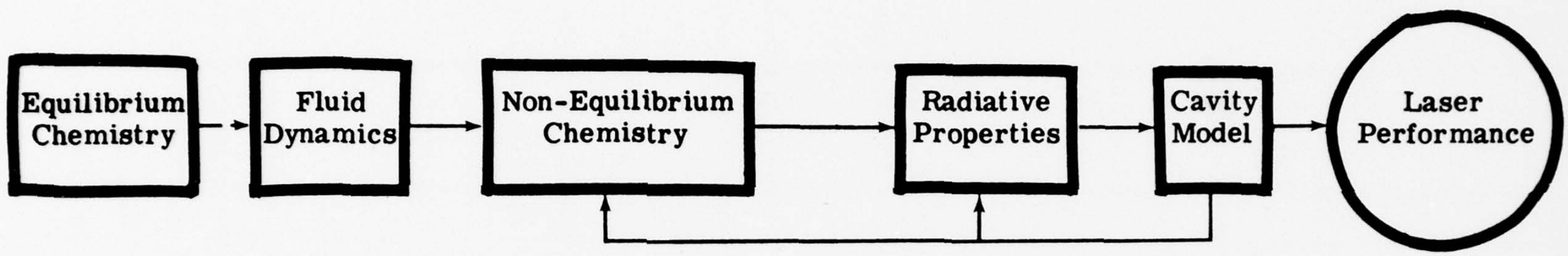

FIGURE 1. $HCl-H_2$ LASER MODELING APPROACH

MERADCOM non-equilibrium chemistry code which was revised and expanded under this contract. Our summary and recommendations appear in the final section of this report. The appendices contain tabular linewidth results and listings of the codes generated.

SECTION 2
LINEWIDTH MODELING

The basic quantity required for analyzing a laser system is the local gain of the medium. This is given as:

$$\alpha = \frac{hN_A}{4\pi}\omega\varphi\rho B(2J + 1)$$

$$\times \left[\frac{n(v + 1)}{Q_{rot}(v + 1)} \exp\left(-\frac{hcE_{v+1, J-1}}{kT}\right) - \frac{n(v)}{Q_{rot}(v)} \exp\left(-\frac{hcE_{v, J}}{kT}\right)\right] \quad (1)$$

The notation is as given by Emmanual [1]. All quantities in this equation are simple functions of the energy levels of the molecule except vibrational state concentrations (n(v), n(v + 1)), the line profile (φ), and the Einstein coefficient (B). Of interest here is the line profile; the Einstein coefficient is discussed in a later section, and the state concentrations are determined by the chemistry.

The detailed line profile depends in a complicated manner on the Doppler and Lorentz linewidths of the particular laser transition; however, for the case in which the Lorentz width is significantly greater than the Doppler width, the line center gain value is simply inversely proportional to the linewidth.

$$\varphi(\omega_c) = \frac{1}{\pi\gamma_{LR}} \quad (2)$$

The Lorentz (or collision-broadened) linewidths are related to the interactions of the lasing molecules with other molecules in the medium. Semi-classically, Lorentz broadening results from collisions undergone by the

lasing molecule which interrupt the lasing process. These collisions may be with either similar or different species than lasing species. In the case of HCl lasing, other HCl molecules are very effective in causing Lorentz broadening because of the relatively large value of the HCl dipole moment and the long-range nature of the dipole-dipole force. On the other hand, homonuclear molecules such as H_2 and atoms are less effective broadening agents because they have no dipole moment.

The basic equation for the Lorentz linewidth is

$$\gamma(m) = \frac{n\bar{v}}{2\pi c}\sum_{J_p} \rho_{J_p}(m)\sigma_{J_p}(m) \tag{3}$$

In this equation, γ is the half-width for a particular rotational transition designated by m. The critical variables in (3) are the rotational populations of the perturbing molecular states ρ_{J_p}, and the broadening cross-sections of the perturbing rotational states σ_{J_p}. For the present discussion, we will consider vibrational states of the perturbing molecules as separate species.

The rotational population ρ_{J_p}, is only a function of the rotational energy levels, the kinetic temperature, and the degeneracies of the rotational states of the perturbing molecules. The critical and difficult factor is the effective broadening cross-section, σ_{J_p}. This can be expressed as [2]

$$\sigma_{J_p} = \pi\left[b_o^2 + C_1 b_o^{-2}\sum_i g_{1i}F_1(k_o) + C_2 b_o^{-4}\sum_i g_{2i}F_2(k_o) + C_3 b_o^{-6}\sum_i g_{3i}F_3(k_o)\right] \tag{4}$$

In (4), b_o is an impact parameter obtained from the solution of the following equation.

$$b_o^2 = \sum_{J_i, J_p} \left\{ C_1 b_o^{-2} \sum_i g_{1i} f_1(k_o) + C_2 b_o^{-4} \sum_i g_{2i} f_2(k_o) \right.$$

$$\left. + C_3 b^{-6} \sum_i g_{3i} f_3(k_o) \right\} \quad (5)$$

In Equations (4) and (5), the C_i are coefficients related to the molecular moments of the molecules, g_{ji} represents Clebsch-Gordan coefficients between molecular states, and the F_i are resonance functions. The F_i describe strengths of various interactions as functions of the energy defect in the rotational energy exchange in the collision process. The F_i approach 1 when the energy defect is small because of resonance between rotational transition energies in the emitting and perturbing molecule.

The multipole moment parameters are contained in the C_i expressions.

$$C_1 = \frac{4}{9} \frac{\left(\mu_1^2 \mu_2^2\right)}{(h\bar{v})^2} \quad (6)$$

$$C_2 = \frac{4}{45} \frac{\left(\mu_1^2 Q_2^2 + \mu_2^2 Q_1^2\right)}{(h\bar{v})^2} \quad (7)$$

$$C_3 = \frac{1}{25} \frac{Q_1^2 Q_2^2}{(h\bar{v})^2} \quad (8)$$

where μ_i and Q_i are the dipole and quadrupole moments of the molecules, and subscripts 1 and 2 refer to the active and perturbing molecules respectively.

2.1 HCl SELF-BROADENED LINEWIDTHS

Values for ρ_{J_p} and σ_{J_p} calculated for the self-broadening of the HCl $P_2(5)$ laser transition are shown in Figure 2. The σ_{J_p}'s presented as bars

are typical of self-broadening where, because of the close match between the rotational energy levels of the molecules, large broadening cross-sections occur for J_p's near transition J values. Large linewidth values result when large cross-sections coincide with large values of the distribution function. For moderate J transitions, the self-broadened cross-sections are generally much larger than the kinetic theory (or hard sphere) cross-sections of the molecules. Compare the HCl kinetic cross-section of $\sim 3 \times 10^{-15}$ cm^2 with the broadening cross-sections plotted in Figure 2. Under these conditions, the Anderson theory used here is reliable. Figure 3 shows good agreement for all temperatures measured [3].

Since the initial states of most lasing transitions are sparsely populated at equilibrium conditions for moderate temperatures, direct measurement data of the line-broadening coefficients for these transitions are difficult to obtain. Thus, knowledge of these linewidths must be based on calculations. A number of interesting factors come into play when we consider these linewidths.

Temperature dependence of individual linewidths is influenced mainly by the broadening molecule's population distribution. Low temperatures result in a population distribution which is sharply peaked near low J_p values. For the self-broadening cases, this means that large ρ_{J_p} values coincide with large σ_{J_p} values at small m. A distribution of linewidths peaked for small m results, as in the curves shown in Figure 3. At higher temperatures, the population distribution is broader, and the linewidths have a weaker m dependence.

Since the rotational constant (B_v) of a molecule changes as a function of the vibrational state, the rotational resonances shift in the higher vibrational states. The effects of these shifting resonances on the linewidths are shown in Figures 4 and 5. The widths for the $1 \rightarrow 0$ bands closely follow the shape of the Boltzmann distribution function ρ_{J_p}. This is because there is

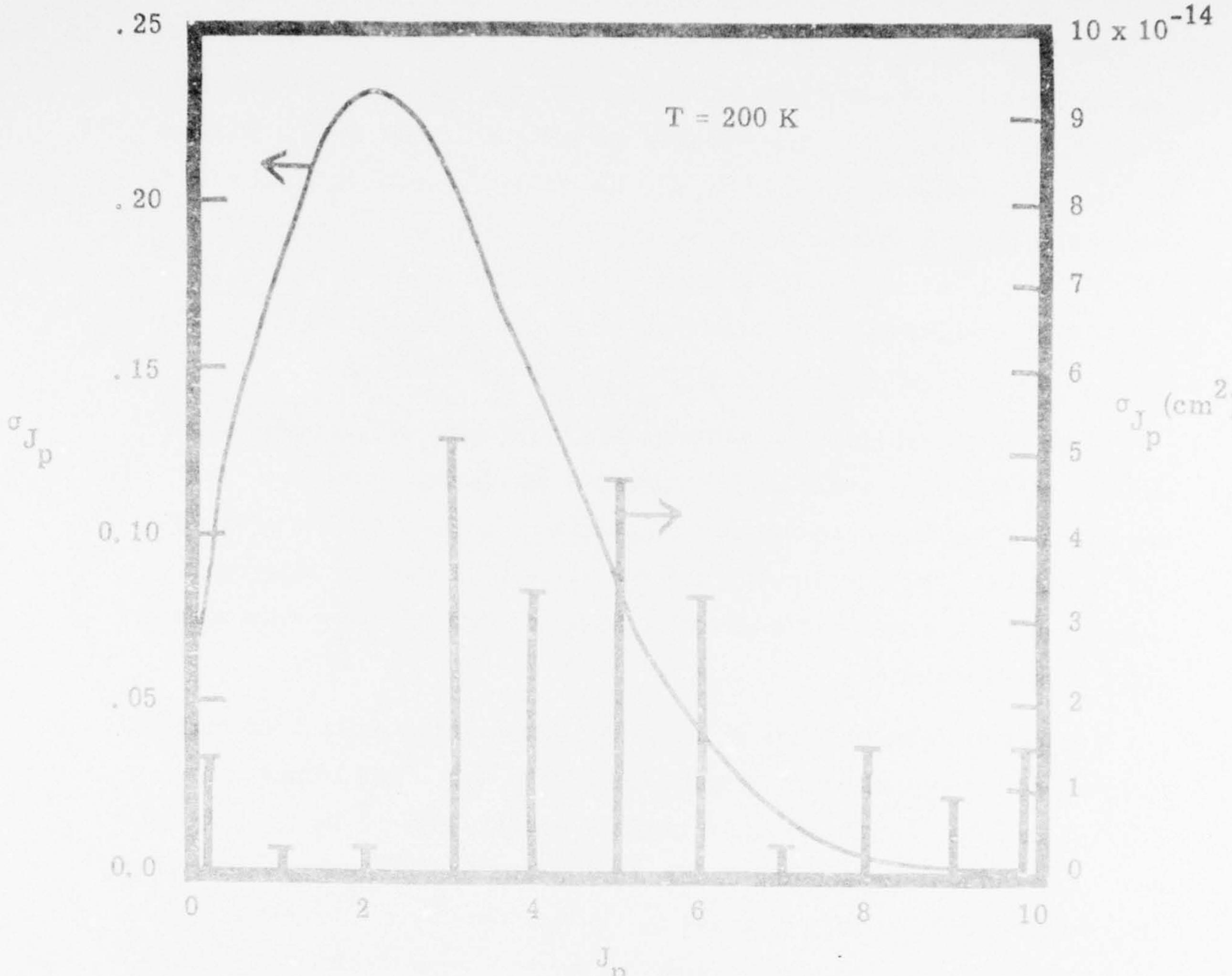

FIGURE 2. CALCULATED POPULATION J_p DISTRIBUTION AND BROADENING CROSS-SECTIONS FOR HCl $P_2(5)$ BROADENED BY HCl (v = 0)

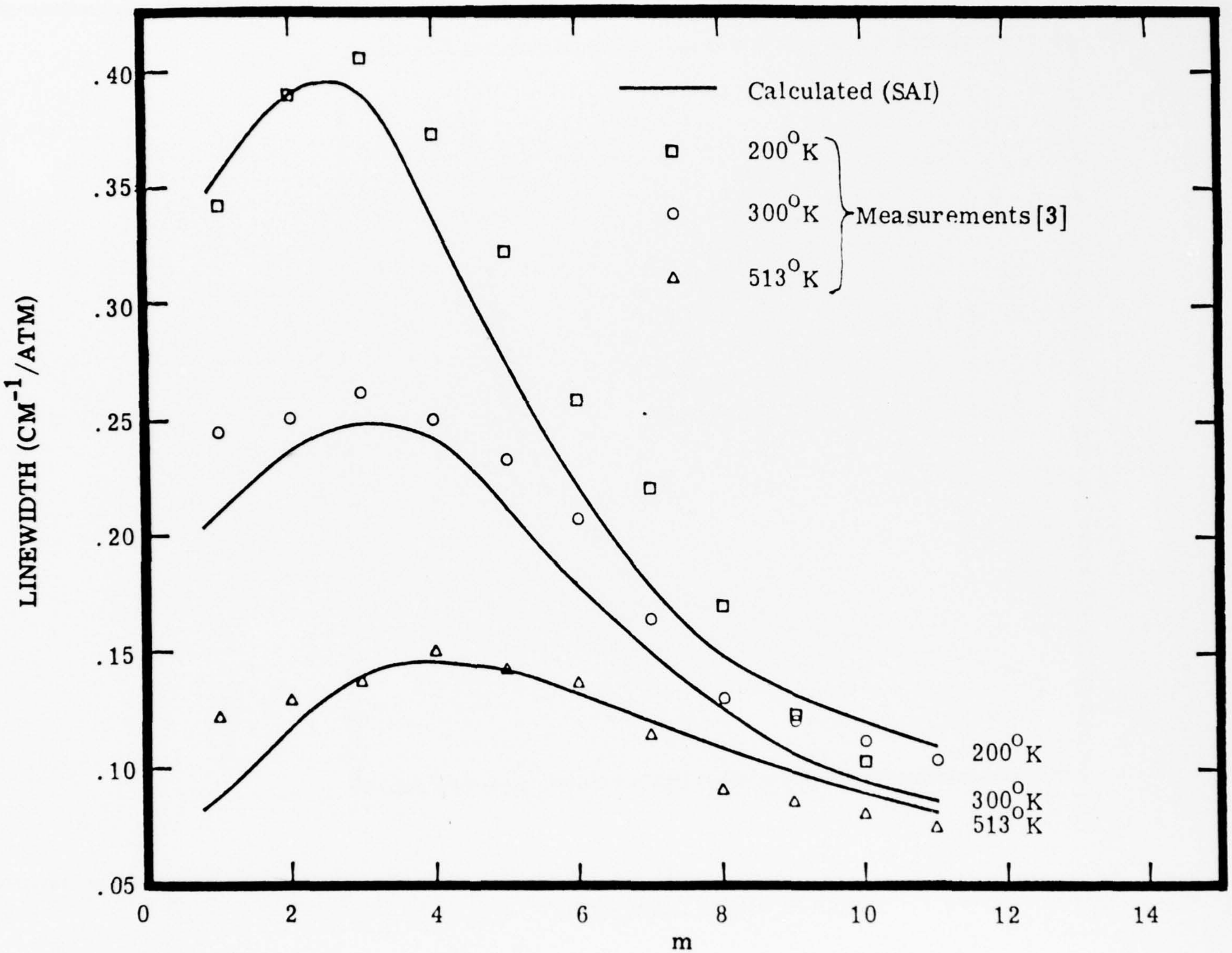

FIGURE 3. COMPARISON OF MEASURED AND CALCULATED LINEWIDTHS FOR HCl ($v = 1 \rightarrow 0$) BROADENED BY HCl ($v = 0$)

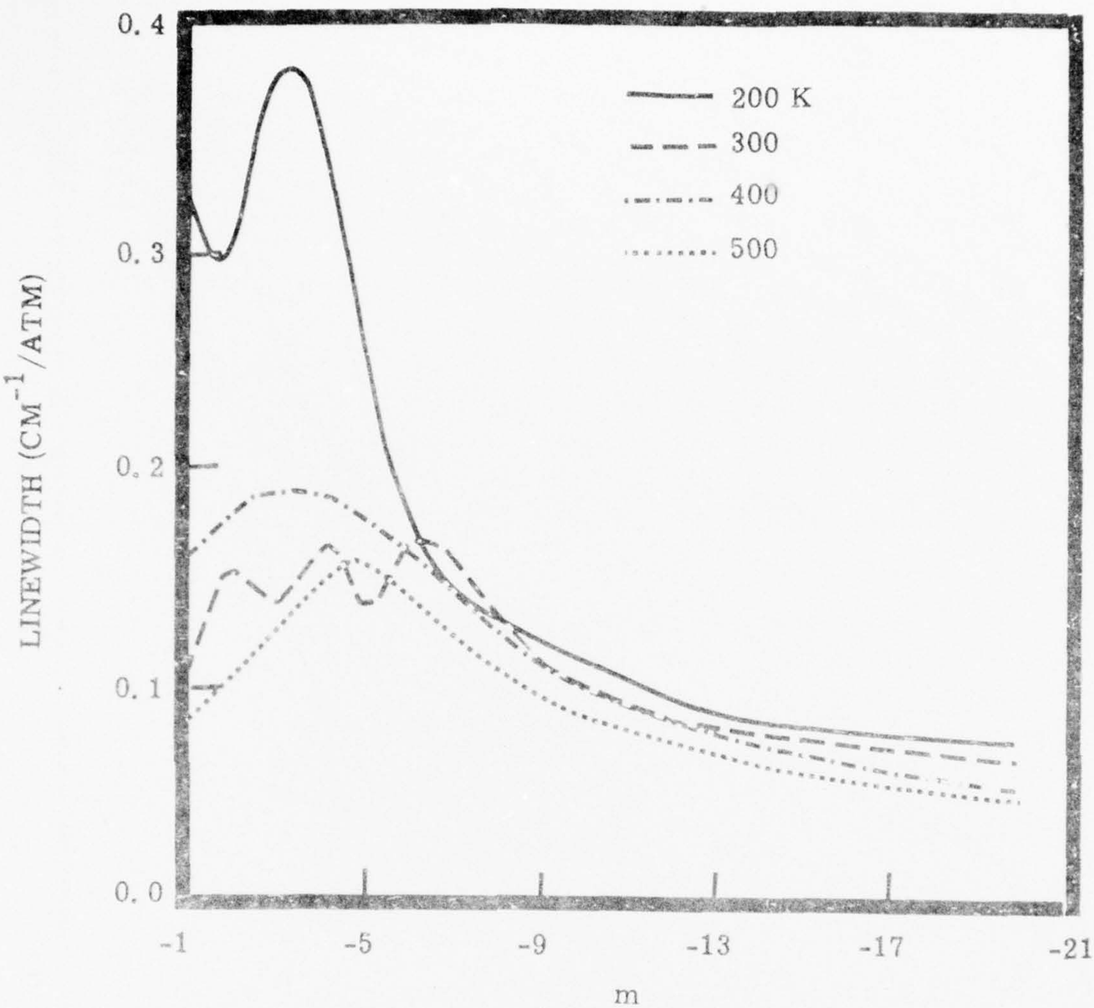

FIGURE 4 CALCULATED LINEWIDTHS FOR THE HCl (v = 2 → 1) LINES BROADENED BY HCl (v = 0) AT VARIOUS TEMPERATURES

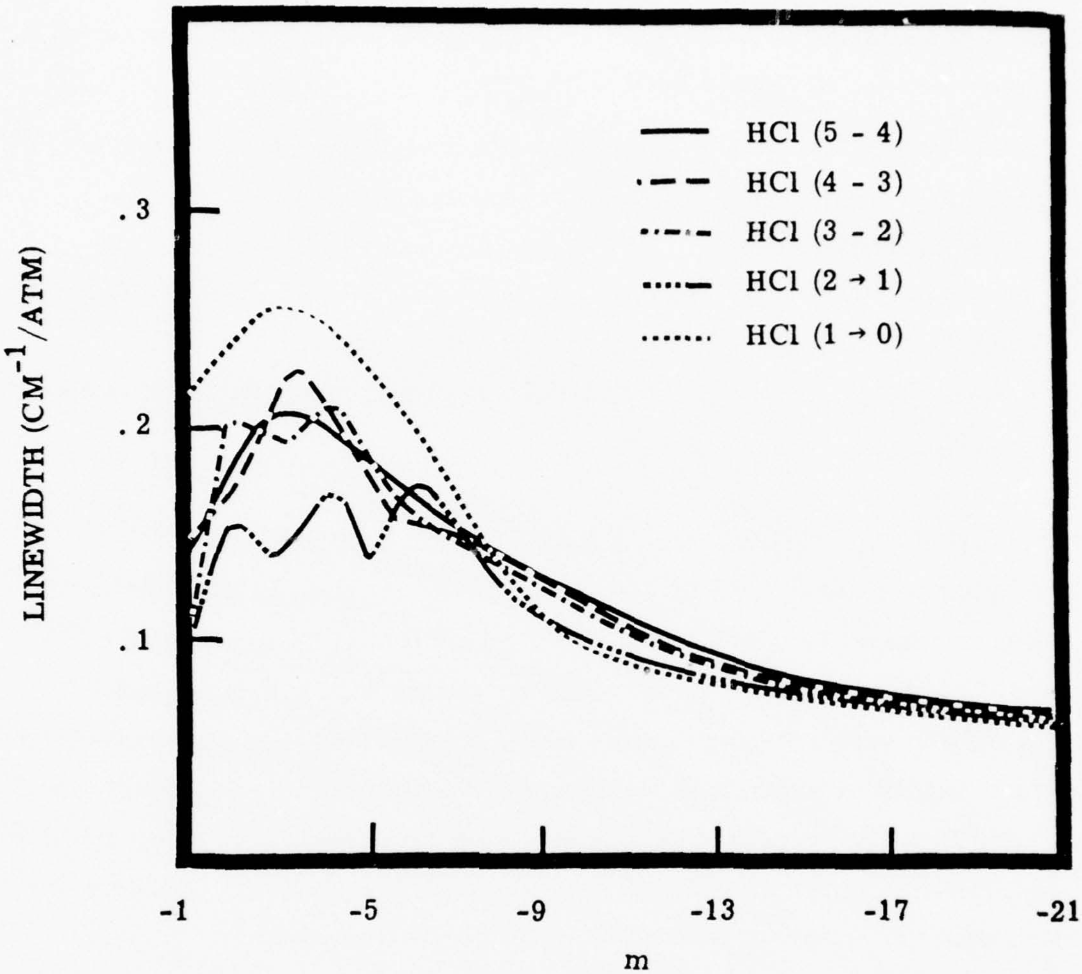

FIGURE 5. CALCULATED LINEWIDTHS FOR VARIOUS HCl VIBRATIONAL TRANSITIONS BROADENED BY HCl (v = 0) AT 300 K

a close match between the resonances in the broadening molecule (HCl (v = 0)) and the active transitions (HCl (v = 1 → 0)). On the other hand, a beat phenomena is observed in the linewidths for the HCl (v = 2 → 1) band because of the shifting resonances between these transitions and the broadening molecules for various rotational states.

Similar resonance effects occur when the broadening by different vibrational states of HCl are considered. This can be seen in Figure 6, where the broadening of the HCl (2 → 1) band by various HCl vibrational states is shown. This figure illustrates the strength of resonance interaction effects for low m values; factors of two differences are calculated for the effectiveness of various HCl vibrational states in broadening the same lasing transition.

2.2 FOREIGN-BROADENED HCl LINEWIDTHS

The principle foreign broadener in the NRML system is H_2. We used the basic approach described in 2.1 to calculate the H_2 broadening of HCl; however, the problem is not as straightforward as with self-broadening. The difficulties with a first-principle calculation of these foreign-broadened widths are that the interactions are weaker, resonances are less likely to occur, and thus the broadening cross-sections are comparable to or smaller than the kinetic theory cross-sections. These problems cause extreme difficulties with the Anderson theory because the small broadening cross-sections imply that the broadening is caused by collisions with impact parameters less than the molecular diameters. The theory, however, assumes straight line trajectories which are unrealistic for small impact parameter collisions. An alternate method for treating these close collisions is critical for calculating foreign broadening linewidths.

Three approaches for treating these close collisions are illustrated in Figure 7. In that figure, b is the impact parameter of the collision, and S(b) is the collision's effectiveness in interrupting the radiative process.

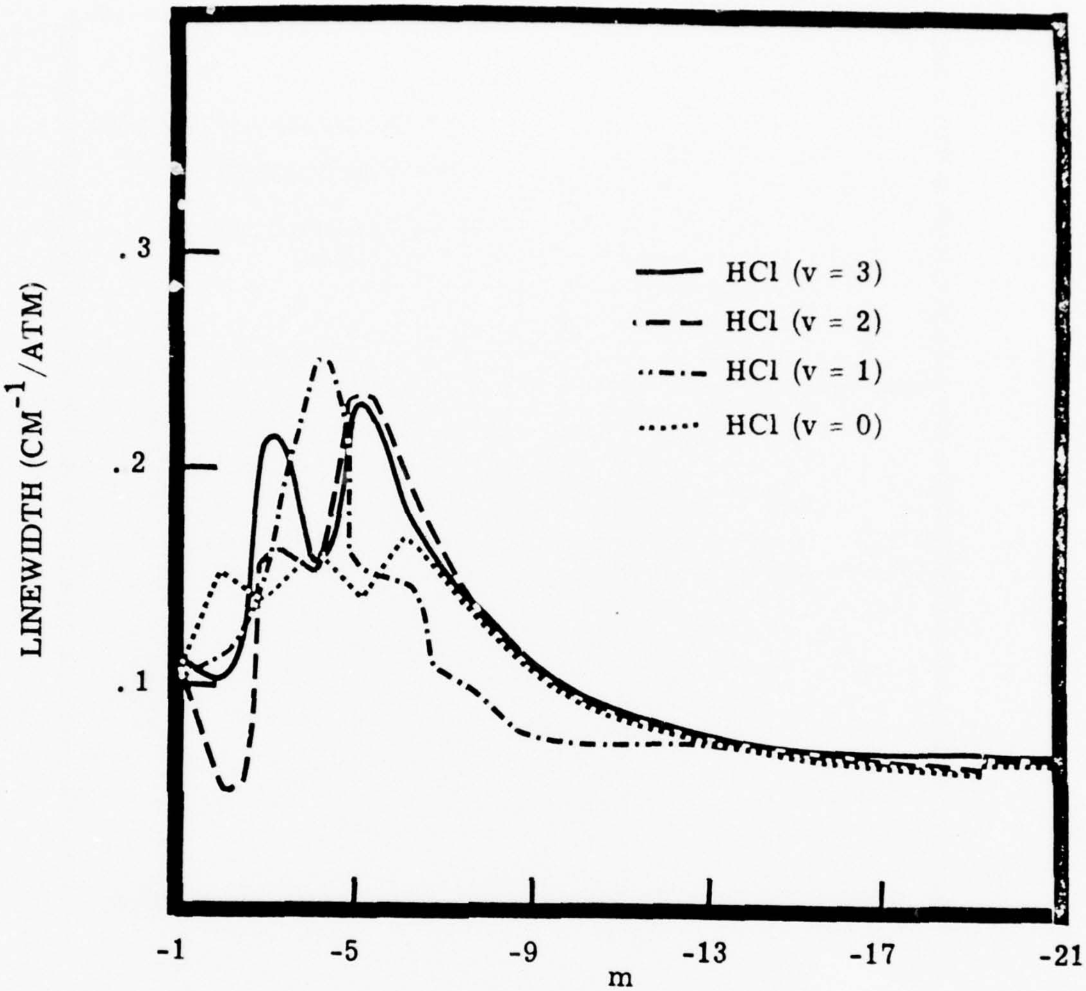

FIGURE 6 CALCULATED LINEWIDTHS FOR THE HCl (v = 2 - 1) LINES BROADENED BY VARIOUS HCl VIBRATIONAL SPECIES AT 300 K

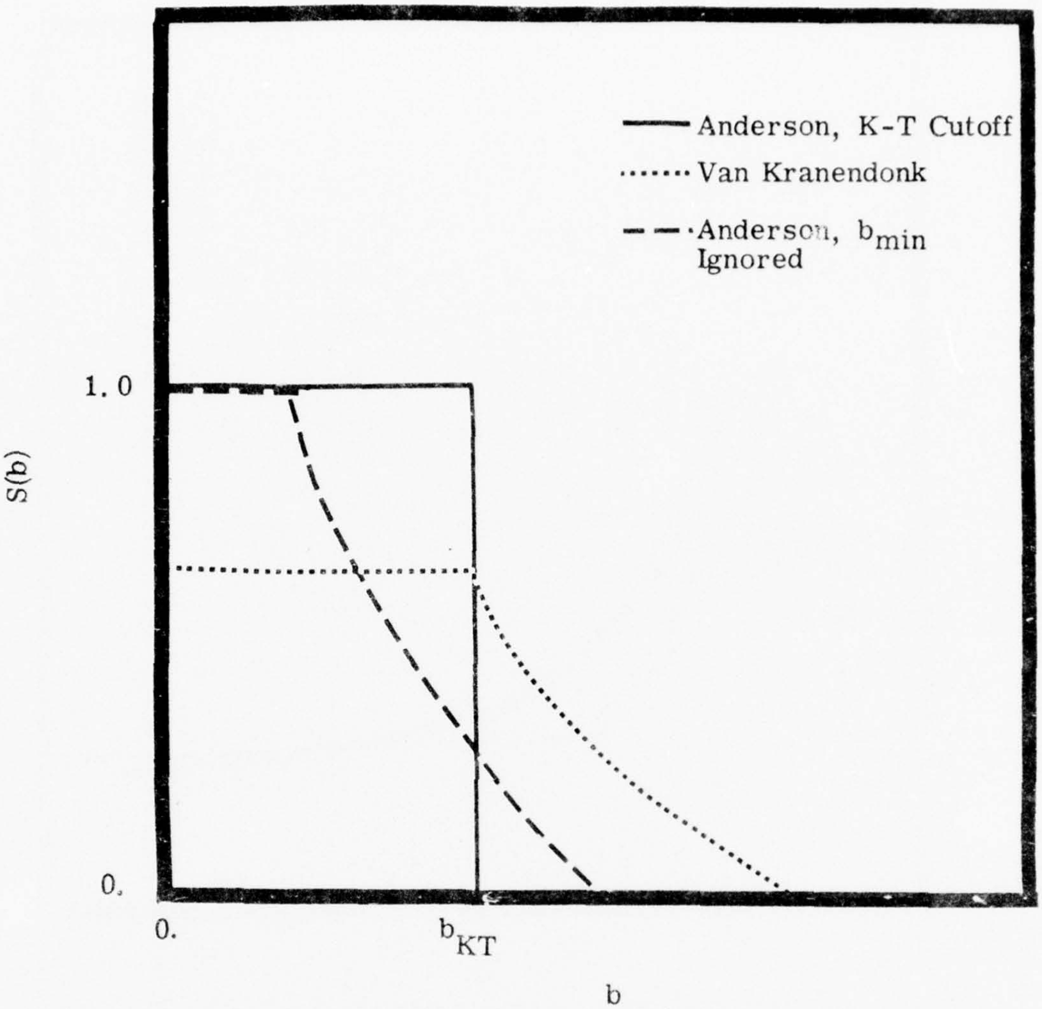

FIGURE 7. APPROXIMATION USED IN THE ANDERSON THEORY FOR SMALL IMPACT PARAMETERS

Anderson's basic approach [4] assumes that any collision with an impact parameter less than the kinetic theory diameter is totally effective in causing broadening. Another approach using the Anderson theory is simply to ignore the unrealistic straight trajectory approximation for close collisions and let the impact parameter be as small as necessary to satisfy Equation 5. In the Van Kranendonk approximation [5], the collision efficiency is calculated at the kinetic theory impact parameter. This collision efficiency is then assumed for all impact parameters smaller than the kinetic theory value.

HCl linewidth computations based on these three assumptions are compared with measurement results in Figure 8. As illustrated here, the basic Anderson theory predicts larger widths than were measured. The Van Kranendonk approach shows reasonable agreement with the measurements for small and large m values but underpredicts the widths for moderate m's. The Van Kranendonk approach fails by underpredicting the cross-sections for small impact parameter collisions.

To fit the data, we use the Van Kranendonk approach but assume that collisions at less than the kinetic theory impact parameter are at least 40% efficient in causing broadening.

The linewidths calculated for HCl broadened by H_2 with the above assumptions are shown in Figure 9. Good agreement is now seen between the calculations and measurements. The predicted hump in the low temperature linewidths near an m of -15 results from a resonance between the radiationless quadrupole transition in H_2 and the dipole transition in HCl. It would be an interesting test of the present theory if experimental data could be obtained at large m value where the hump is predicted. Although small variations in the linewidths may be expected for different vibrational states of the active and perturbing molecules, we have not calculated them in the present study.

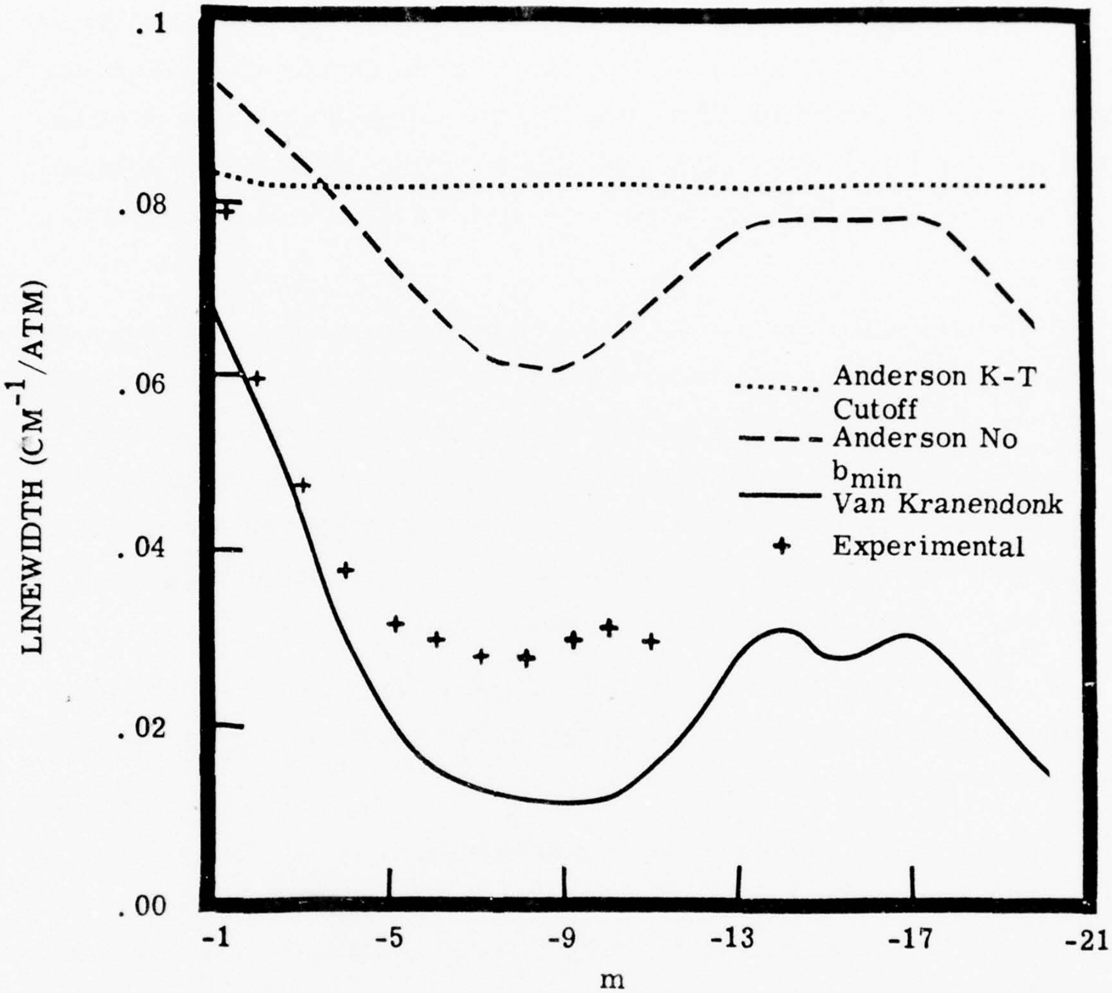

FIGURE 8. COMPARISONS OF EXPERIMENTAL HCl BROADENED LINEWIDTHS WITH VALUES CALCULATED BY VARIOUS METHODS

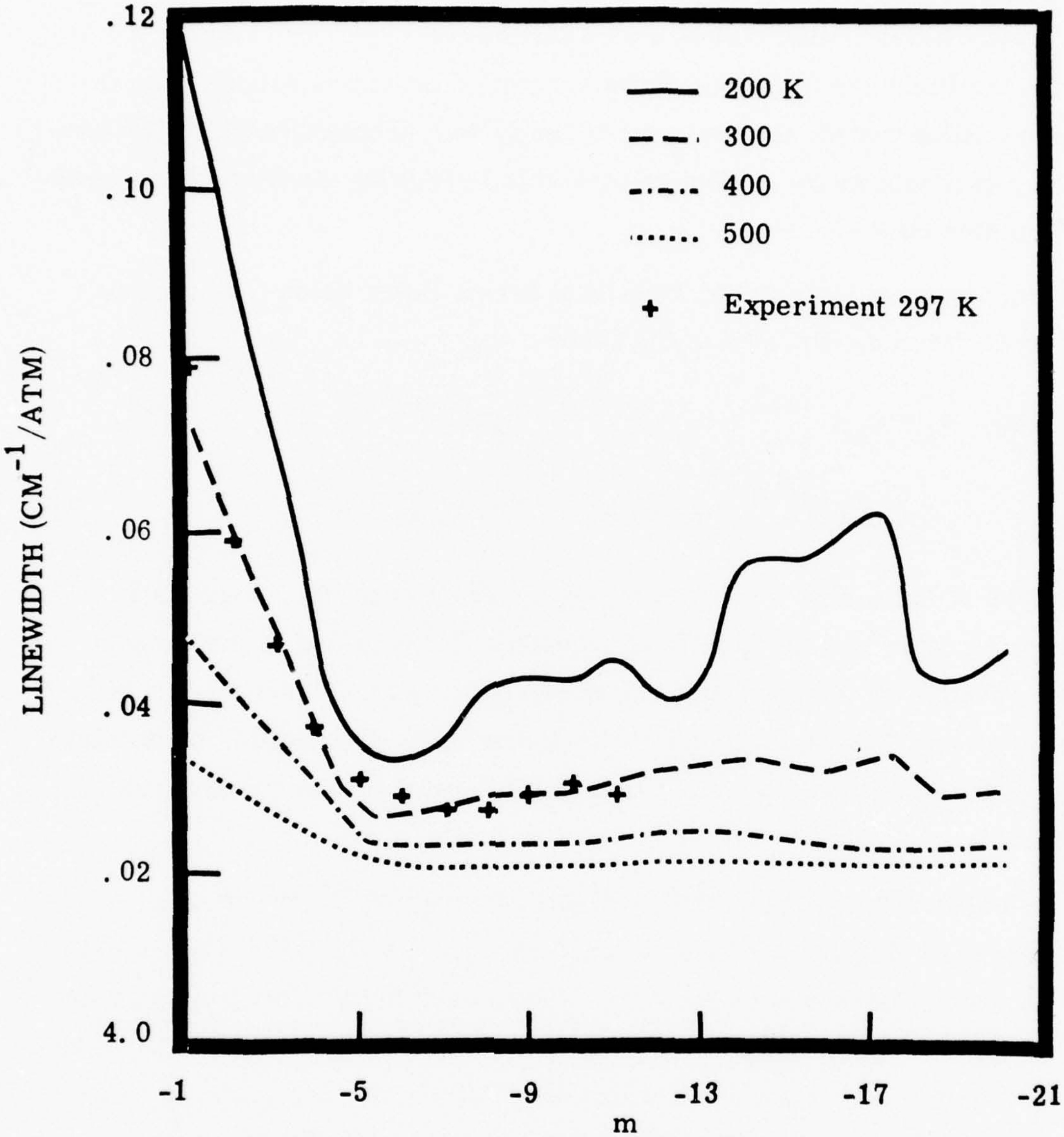

FIGURE 9. HCl (1 → 0) LINEWIDTHS BROADENING BY H_2 (v = 0) AT VARIOUS TEMPERATURES

The linewidths calculated for 300 K for both self-broadening and H_2 broadening of HCl are given in Appendix I.

2.3 LINEWIDTH SUBROUTINE DEVELOPMENT

To facilitate the inclusion of these detailed linewidth calculations in laser modeling codes, a least-square fitting was accomplished of HCl linewidths and a subroutine written to utilize the resulting coefficients in radiative transfer codes.

The series of exponential functional forms listed below was used to represent the m dependence of the linewidths.

$$\gamma(m) = c_1 + c_2 e^{-m/4} + c_3 m e^{-m/4} + c_4 m^2 e^{-m/2} + c_5 m e^{-m^2/8} + c_6 m^2 e^{-m^2/16} + c_7 e^{-m^2/8} \tag{9}$$

This type of expansion works very well for linewidths [6]. Figures 10 through 12 represent the quality of computer fits obtained in the present study. Figure 10 is representative of the better fits, Figure 11 is a nominal match and Figure 12 is one of the poorer fits. The poorer ones miss some of the fine detail in the calculations but overall, the results are reasonable.

In addition to fitting the HCl self-broadening and H_2 broadening, experimental linewidths of HCl broadened by Ar were also fit. The experimental widths measured by Petrov [7] were used because they agree with other authors' results at 300 K [8] and also include higher temperature results. We plotted the widths measured by Petrov at 300 and 600 K on log-log paper and assumed a straight line approximation to interpolate or extrapolate values at 200, 400 and 500 K. These linewidths were then fit in the same manner discussed above and the results are shown in Figure 13.

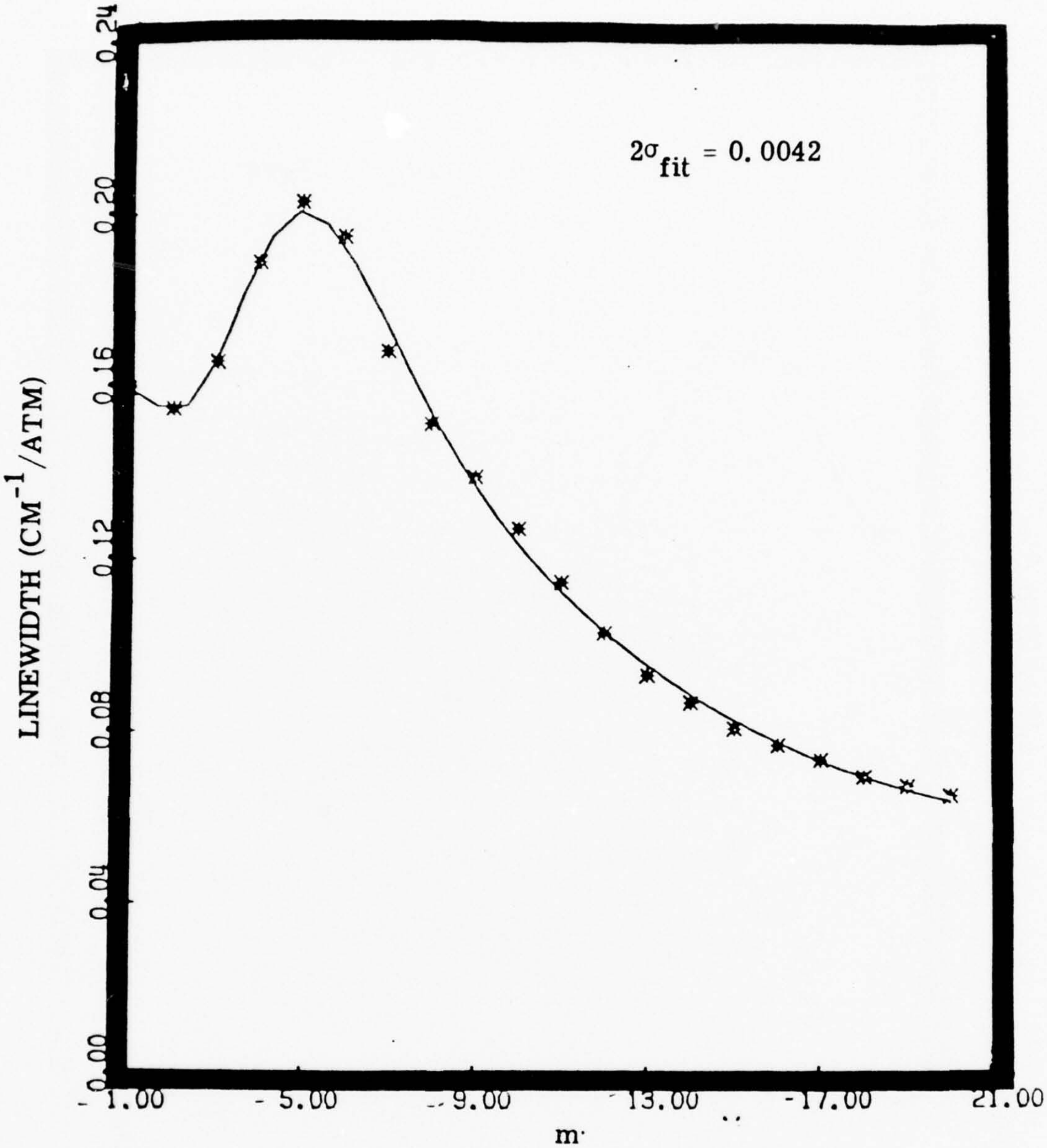

FIGURE 10. LEAST-SQUARE FIT TO HCl (7 → 6) LINEWIDTHS BROADENED BY HCl (v = 0) AT 400 K

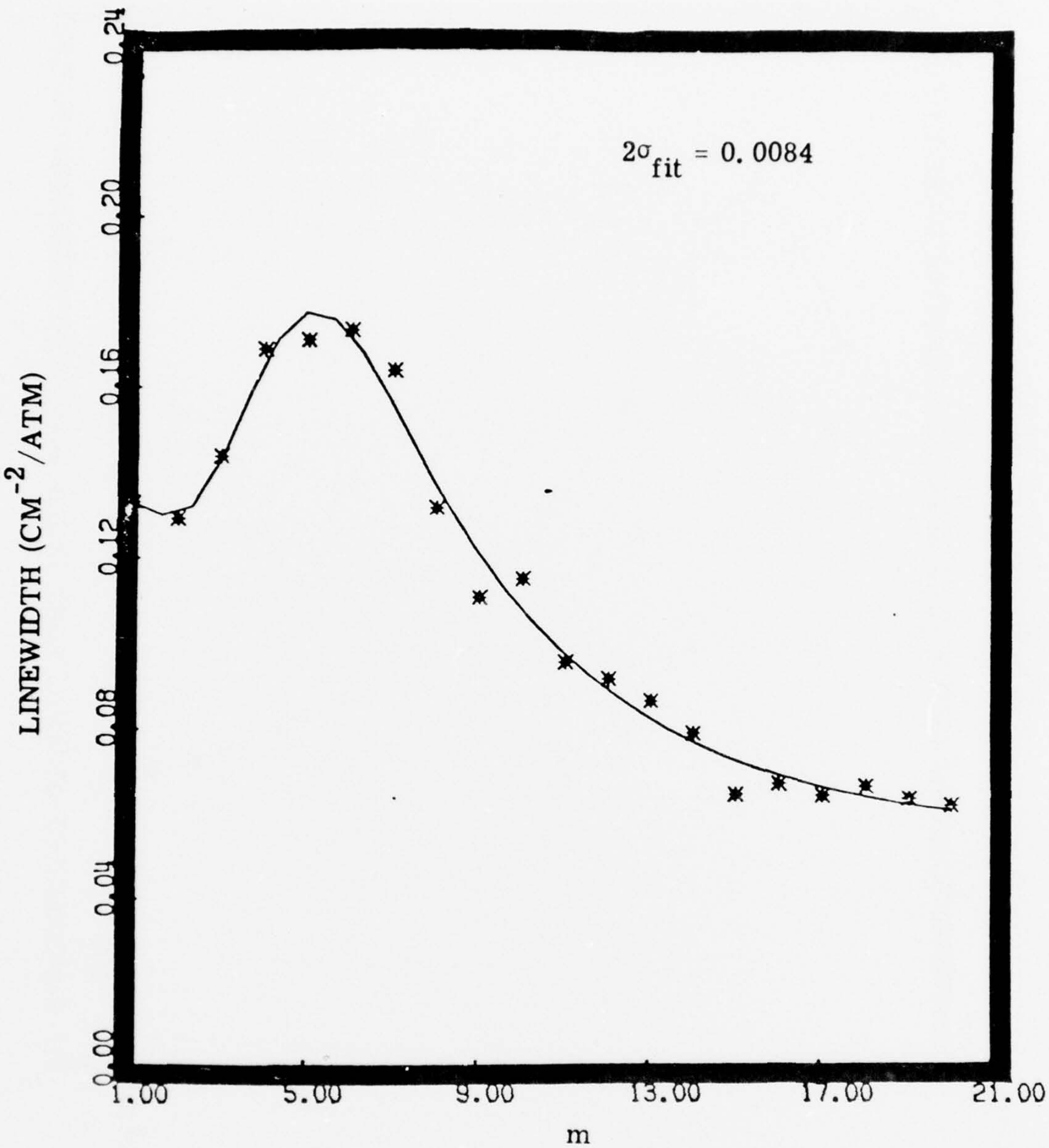

FIGURE 11. LEAST-SQUARE FIT TO HCl (5 → 4) LINEWIDTHS OF HCl (v = 0) BROADENED BY HCl (v = 0) AT 400 K

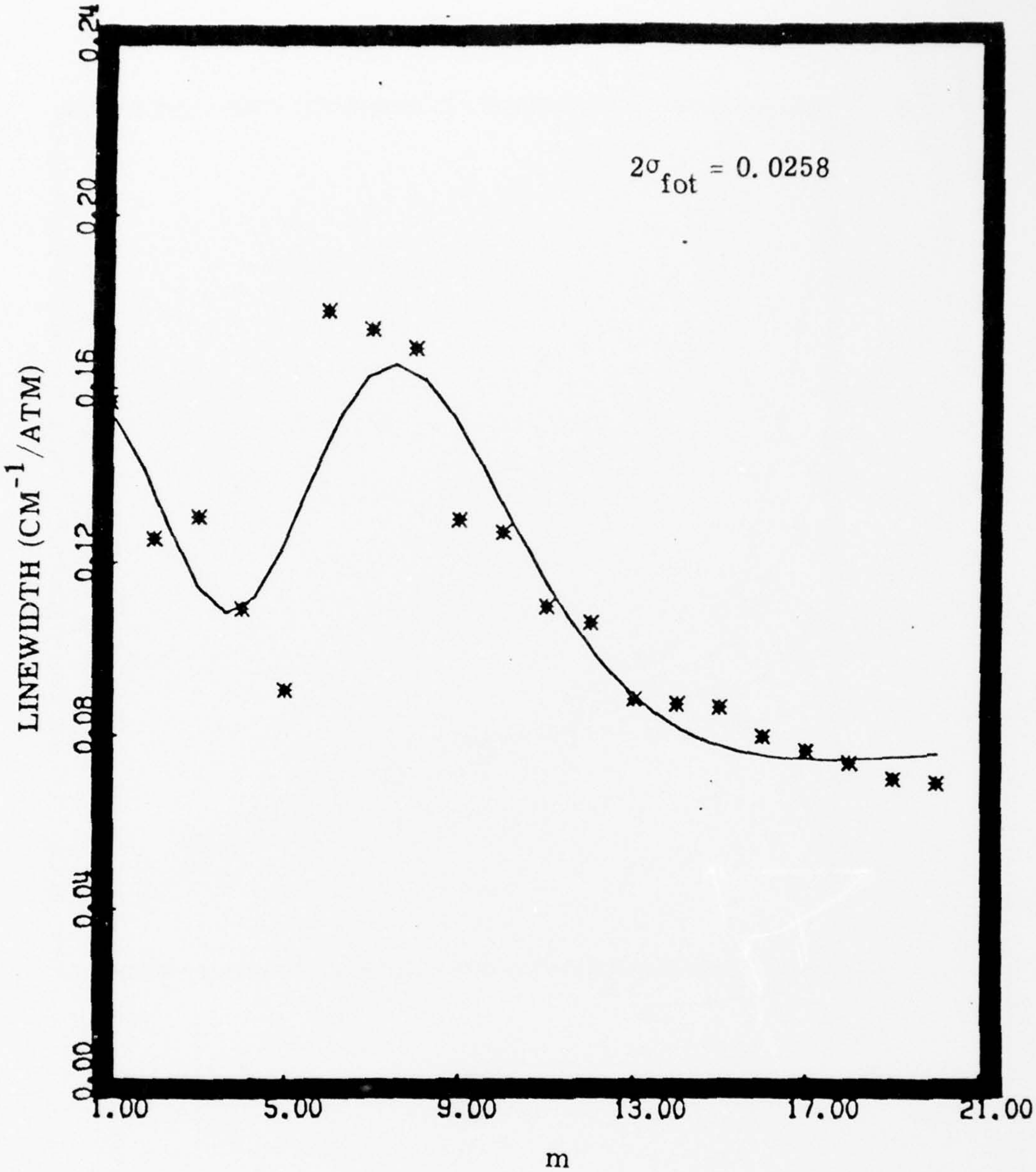

FIGURE 12. LEAST-SQUARE FIT TO HCl (9 → 8) LINEWIDTHS BROADENED BY HCl (v = 0) AT 400 K

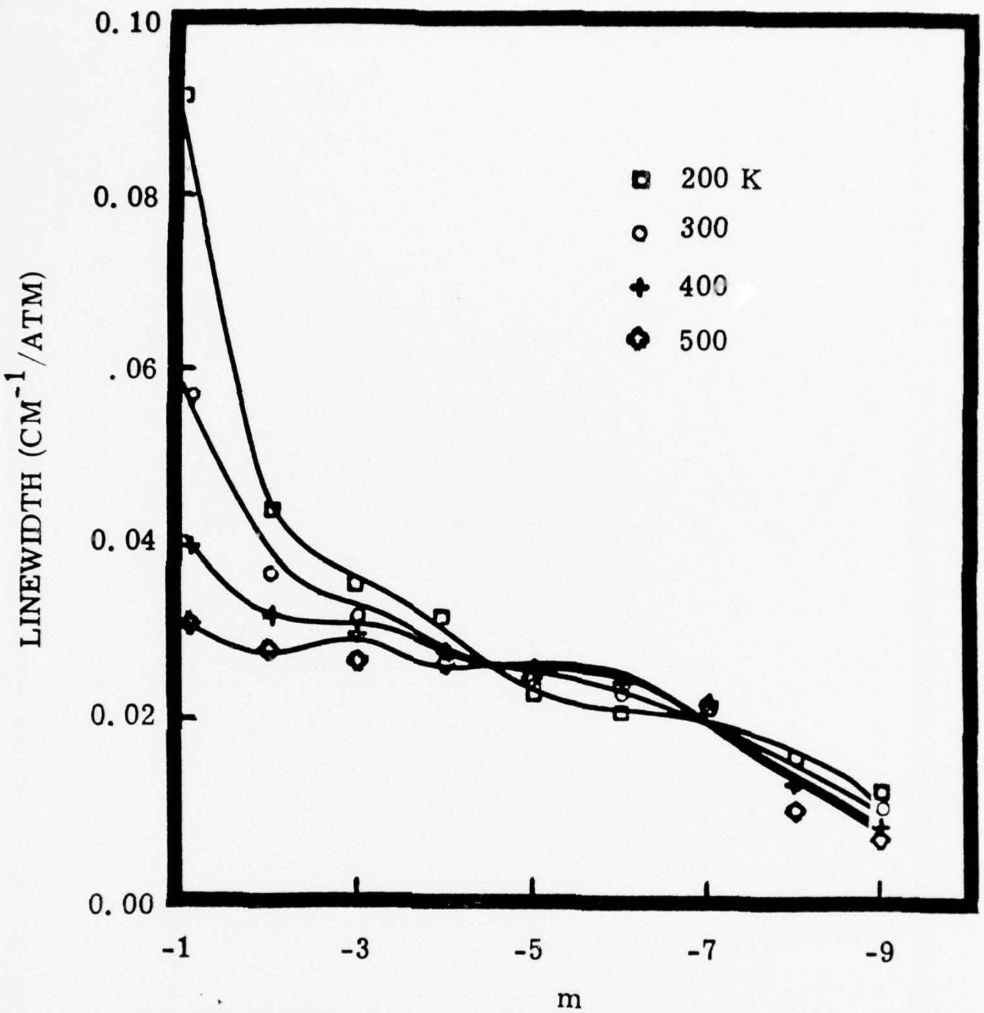

FIGURE 13. LEAST-SQUARE FITS TO HCl LINEWIDTHS BROADENED BY Ar

The least-square fit parameters for all HCl widths form Appendix II.

2.4 LINEWIDTH EVALUATION SUBROUTINE

To make the linewidth results easily assessable to HCl laser modeling groups, we wrote a computer subroutine which uses the least-square fit parameters with the standard chemical variables and returns the computed pressure-broadened linewidth. Table 1 lists the variables required for calling this subroutine and gives the common storage assignments for the least-square parameters. The basic computation done by the program is given as Equation 10.

$$\gamma(T, m) = p\left(\sum_{\substack{i = \text{perturbing} \\ \text{molecular states}}} \rho_i \left(\sum_{\substack{j = \text{fitting} \\ \text{functions}}} f_j(m) C_{ijk}(T) \right) \right) \tag{10}$$

Bookkeeping complications arise because the laser modeling codes may include more or fewer molecular states than are represented in the least-square coefficients, and temperature interpolation is usually required; however, the program includes the more general cases. Appendix III lists the subroutine GAMMA2 along with a calling program and a simple test case.

TABLE 1

CALLING SEQUENCE AND COMMON ASSIGNMENT
FOR LINEWIDTH SUBROUTINE GAMMA2

Calling Sequence

WIDTH = GAMMA2 (PTOT, TKEN, CLS, NCLS, CNLS, NCNLS, CSA, NCSA, LV, M)

Variable	Description
PTOT	Total Pressure
TKEN	Kinetic Temperature
CLS( )	Array of the mole functions of the vibrational states of the lasing species
NCLS	Number of mole fraction in CLS
CNLS( )	Array of mole fractions of the vibrational states of the non-lasing species
WCNLS	Number of mole fractions in CNLS
CSA( )	Array of mole fractions of other species
NCSA	Number of mole fractions in CSA
LV	Vibrational designation of lasing transition
M	Rotational designation of lasing transition ($-J_{final}$)

Common

Variable	Description
NPL	Number of self-broadening states included
NVL	Number of vibrational lasing transitions included
NT	Number of temperatures included
TS( )	Temperatures included
COFT( )	Self-broadening least-square fit coefficients
NPNL	Number of foreign broadening vibrational states
CNOFT( )	Foreign broadening coefficients
NPA	Number of other broadening species
CAOFT( )	Coefficients for other species

SECTION 3
HCl EINSTEIN COEFFICIENTS

The Einstein coefficients of a molecular transition are related to the electric dipole matrix element of that transition by the following formulae:

$$A(v'J' \rightarrow vJ) = \frac{64\pi^4 \nu^3 |m|}{3h(2J' + 1)} |\langle v'J'|\mu(r)|vJ\rangle|^2 \ (\text{molecule-sec})^{-1}$$

$$B(v'J' \rightarrow vJ) = \frac{32\pi^4 |m|}{3h^2 c(2J' + 1)} |\langle v'J'|\mu(r)|vJ\rangle|^2 \left(\frac{\text{cm}^2}{\text{molecule-erg-sec}}\right)$$

$$B(v'J' \leftarrow vJ) = \frac{(2J' + 1)}{(2J + 1)} B(v'J' \rightarrow vJ)$$

Matrix element evaluations for laser transitions often must be extrapolated from matrix elements of other non-lasing transitions which are more accessible to measurement. This procedure was followed in an earlier series of calculations by the present authors on the HCl molecule [9, 10]. In this earlier work, the available experimental determinations of the vibrational matrix elements, $\langle 0|\mu|1\rangle$ and $\langle 0|\mu|2\rangle$, were reviewed and "best" values selected.

Since publication of the earlier work, we have become aware of some additional vibrational matrix element values obtained from dispersion and absorption measurements of gaseous HCl [11, 12, 13]. These additional results are presented in Figure 14 along with the measurement values included in the earlier paper. In that figure, the results of an experimenter who reported values of both matrix elements are represented as a point. Where a particular author has measured only one matrix element, this result is presented as a slash on the appropriate axis.

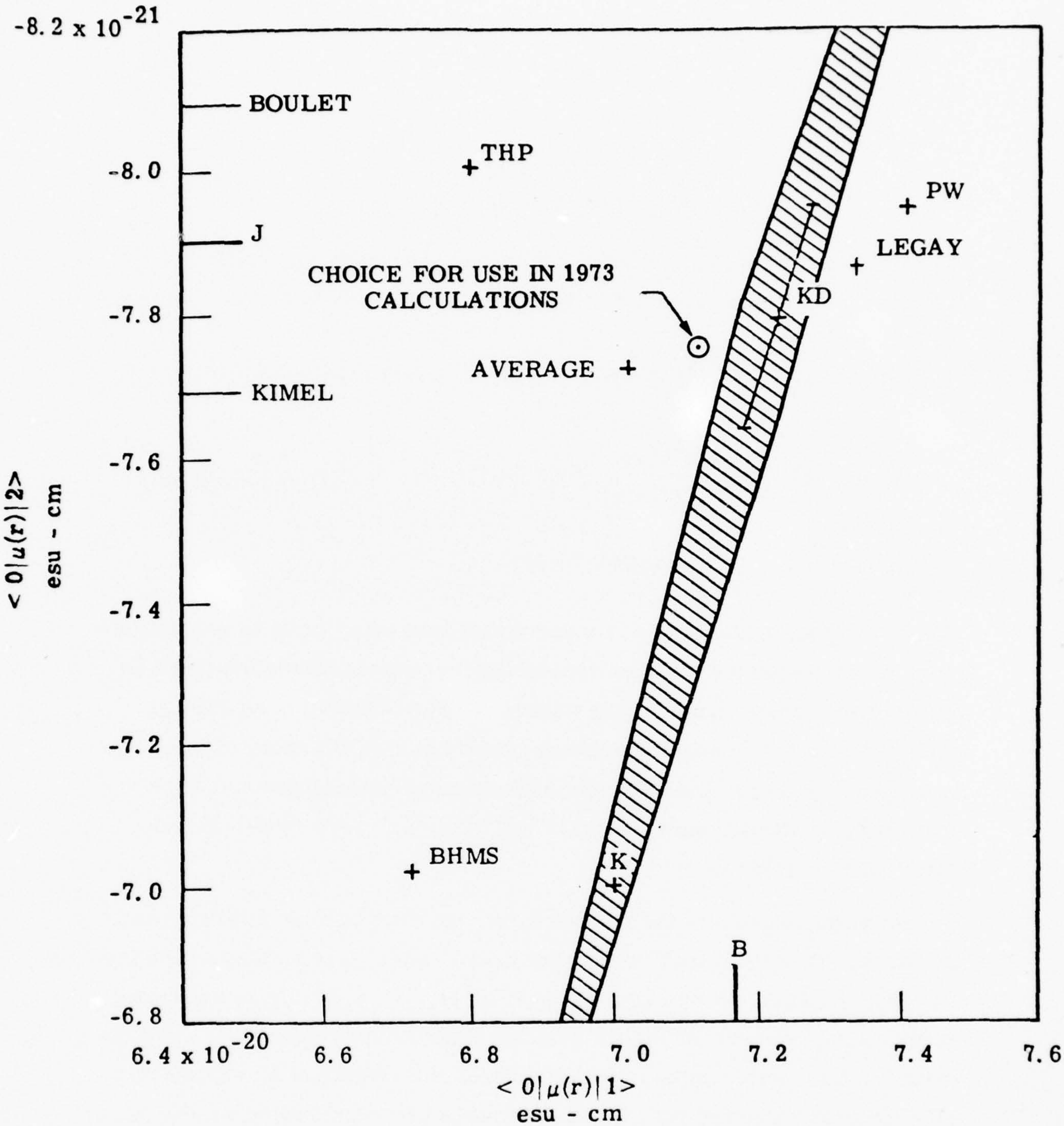

FIGURE 14. EXPERIMENTAL DETERMINATIONS OF $\langle 0|\mu|1\rangle$ AND $\langle 0|\mu|2\rangle$ FOR HCl

The results of Kimel and Legay are seen to agree to within three percent with the values selected for use in the earlier calculations; however, the value obtained by Boulet is nearly 6% larger than the value of $\langle 0|\mu|2\rangle$ previously assumed. When the additional data is considered with the results included previously, no significant trends emerge. Thus, we have decided not to redo the Einstein coefficient calculations in the present study.

SECTION 4
CHEMISTRY CODE DEVELOPMENT

An improved set of finite rate chemistry codes was developed in this program from previous MERADCOM codes. A flow chart of these codes is shown in Figure 15. A list of important variables used in the chemistry routines is given in Table 2. As presently configured, the codes treat up to 99 species including catalytic species, and accept chemical reactions in a manner very similar to standard chemical notation. The codes return the enthalpy change from the chemical reaction and the rates of production of the various species.

The calling program for the chemistry routines is CHEMS. CHEMS first reads the thermodynamic data for each species. These inputs are molecular weight, enthalpy of formation at 25 K, and specific heat and enthalpy as a function of temperature. Next, the reactions to be included are entered and followed by the reaction rate coefficients. A numeric code designates the form of the reaction rates to be used for each reaction. Finally, the flow variables, pressures, temperatures and time increments are entered, and CHEMS calls on additional subroutines to perform the computations.

The housekeeping routines CHEMVT and CHEMSUM compute the variables required for the V-T deactivation processes and for using the composite compounds. Then, the routine CHMSTY is called to compute the species formation rates.

The subroutine CHMSTY first calls the MATH subroutine to compute the reaction rate at the specific temperature of interest. Next, CHMSTY evaluates the individual production rate for each species and each reaction,

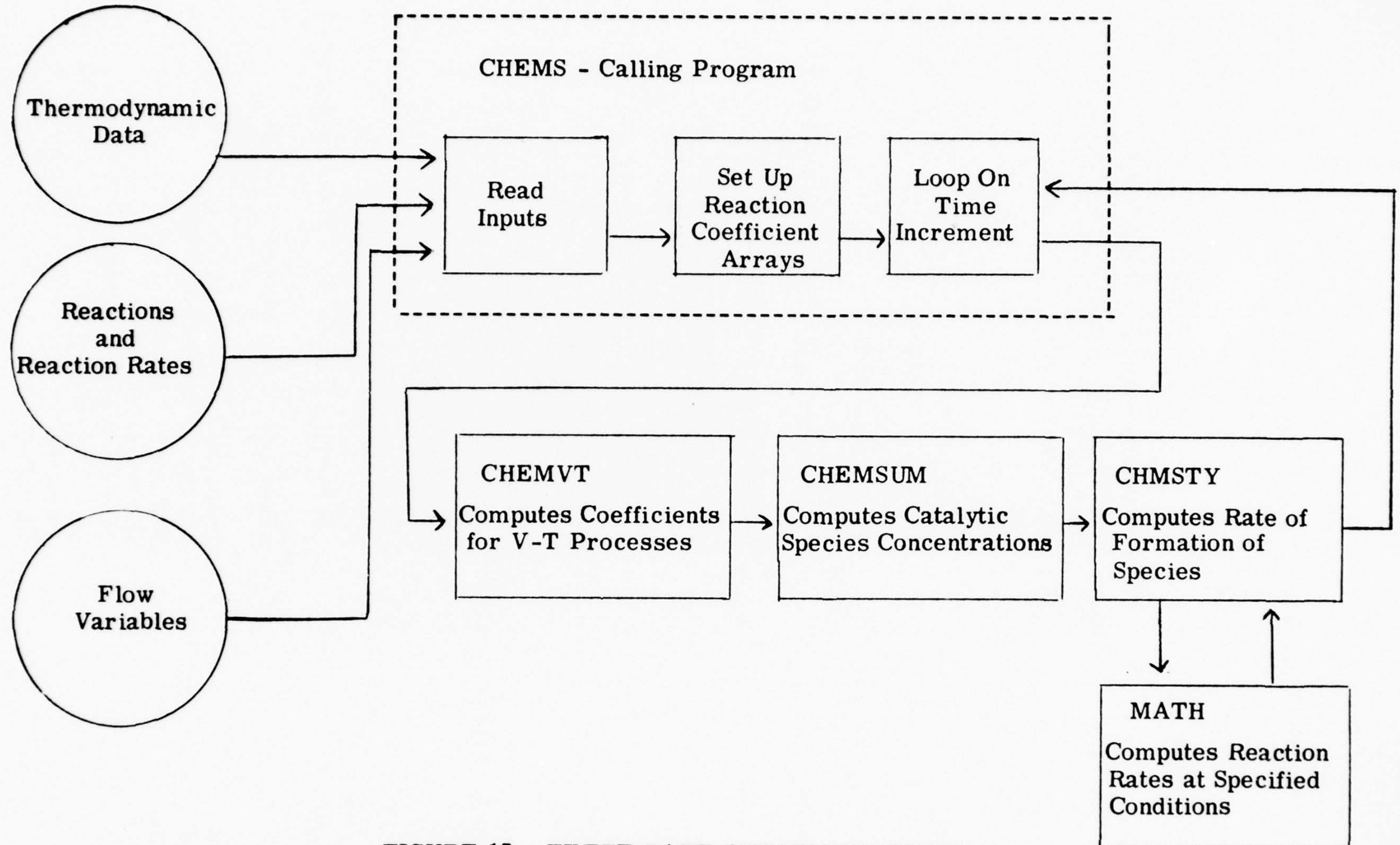

FIGURE 15. FINITE RATE CHEMISTRY CODES

TABLE 2

DEFINITIONS OF PARAMETERS USED IN CHEMISTRY ROUTINES

Variable	Description
AID	Equivalent to SPECIE (in common)
ALPHA	Concentration
AT	Throat area
AVAGAD	Avagados number
A, A1, A2	Areas
AR	Area ratio
CN	Concentration
CNU	Concentration
CNTI	Total mole fraction
CPTB	Specific heat table
CP, CP1, CP2	Specific heat table
DT	ΔTime
DTEMP	Δ Temperature for convergence check & extrapolation
DTMIN	ΔTemperature for convergence
DH	ΔH - enthalpy
DH1	ΔH - enthalpy due to chemistry
DH2	ΔH - enthalpy due to radiation
DX	Axial increment (mm) input
DM	ΔMach number
C0-C3	Temporary constants
DMW	ΔMolecular weight
G	Gibbs Function
GTB	Gibbs Function Table
GAMA, GAMA1, GAMA2	Ratio of specific heats
HF	Enthalpy of formation
HTB	Enthalpy Table
IBLANK	Blank field
IFLAG	Write control
IL, IR	Stoichiometric reaction coefficients
IMAX	Number of axial elements in the expansion region
JMAX	Number of axial elements in the cavity region
MWT	Molecular weight table
NALL	Number of catalytic species
NRT	Number of reactions
NST	Number of species
NT	Number of temps in table
R	Gas constant
P, P1, P2	Pressure
T	Temperature

and sums the values to get the total species production rates. These values are then returned to CHEMS which increments the species concentrations by the necessary amount and sets up for the next step.

A listing of the current versions of these codes is given in Appendix IV. The codes have been run with the input data listed in Appendix V; the code results have been compared with a non-lasing run with the PSI code. There was good agreement with the PSI code results for this case; however, the present code should be compared with a more thorough set of calculations before it is assumed to be totally valid.

SECTION 5

SUMMARY AND RECOMMENDATIONS

In the present program, a set of general purpose subroutines has been developed for use in laser modeling codes. These subroutines provide easy access to collisional linewidth data for the HCl - H_2 laser system and a general set of finite rate chemical kinetics routines. Also, the linewidth and Einstein coefficient data relevant to the HCl - H_2 laser system have been reviewed and revised.

Depending on MERADCOM's current interest and priorities, the present study suggests three possible actions:

1) continue the development of state-of-the-art subroutines with the implementation of finite element methods for solution of the coupled gas dynamics and radiative flow equations in the laser model,

2) incorporate the present subroutines with presently available radiative and fluid flow routines to evaluate the HCl - H_2 laser experimental results and predict ultimate laser performance, and

3) measure or analyze linewidth and Einstein coefficient data for other laser systems and format these results for use in the codes developed here.

These programs could be implemented either sequentially or simultaneously in the coming fiscal year. In any event, pursuance of these programs would contribute to MERADCOM's ability to accurately model and evaluate high-energy laser concepts and devices.

APPENDIX 1

SELECTED LINEWIDTH CALCULATION RESULTS FOR 300 K

CALCULATED HALF-WIDTHS FOR HC10 PERTURBED BY HC-0 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 10.136340 BE(F) = 10.440470 BE(P) = 10.440470
MU(HC10) = 1.123E-18 MU(HC-0) = 1.108E-18
Q(HC10) = 7.600E-26 Q(HC-0) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	2.169063E-01	2.788841E-14
-2	2.451867E-01	3.152451E-14
-3	2.634863E-01	3.387736E-14
-4	2.579104E-01	3.316044E-14
-5	2.323908E-01	2.987929E-14
-6	1.951782E-01	2.509474E-14
-7	1.637262E-01	2.105085E-14
-8	1.367220E-01	1.757883E-14
-9	1.185068E-01	1.523684E-14
-10	1.043747E-01	1.341982E-14
-11	9.587073E-02	1.232644E-14
-12	8.892447E-02	1.143334E-14
-13	8.439416E-02	1.085086E-14
-14	8.040339E-02	1.033775E-14
-15	7.703322E-02	9.904431E-15
-16	7.454288E-02	9.584246E-15
-17	7.191777E-02	9.246720E-15
-18	7.044119E-02	9.056869E-15
-19	6.866419E-02	8.828397E-15
-20	6.786400E-02	8.725513E-15

CALCULATED HALF-WIDTHS FOR HC21 PERTURBED BY HC-0 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 9.334431 BE(F) = 10.136340 BE(P) = 10.440470
MU(HC21) = 1.152E-18 MU(HC-0) = 1.108E-18
Q(HC21) = 7.600E-26 Q(HC-0) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	9.919763E-02	1.275419E-14
-2	1.540290E-01	1.980404E-14
-3	1.399596E-01	1.799509E-14
-4	1.663214E-01	2.138452E-14
-5	1.395081E-01	1.793705E-14
-6	1.732100E-01	2.227022E-14
-7	1.590666E-01	2.045176E-14
-8	1.223545E-01	1.573155E-14
-9	1.052846E-01	1.353682E-14
-10	1.014142E-01	1.303918E-14
-11	9.173584E-02	1.179480E-14
-12	9.349430E-02	1.202089E-14
-13	8.667868E-02	1.114459E-14
-14	8.333015E-02	1.071405E-14
-15	7.831699E-02	1.006949E-14
-16	7.430738E-02	9.553962E-15
-17	7.340944E-02	9.438512E-15
-18	7.104200E-02	9.134125E-15
-19	6.978709E-02	8.972769E-15
-20	6.829933E-02	8.781550E-15

CALCULATED HALF-WIDTHS FOR HC32 PERTURBED BY HC-0 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

```
BE(I) =   9.534647 BE(F) =   9.834431 BE(P) = 10.440470
MU(HC32) =      1.161E-18 MU(HC-0) =      1.708E-18
Q(HC32) =     7.600E-26 Q(HC-0) =     7.600E-26
B(MIN) =     3.100E-08
```

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.167527E-01	1.501131E-14
-2	1.991665E-01	2.560754E-14
-3	1.949963E-01	2.507136E-14
-4	2.099559E-01	2.699476E-14
-5	1.780857E-01	2.289710E-14
-6	1.594561E-01	2.050183E-14
-7	1.341285E-01	1.724536E-14
-8	1.232594E-01	1.584790E-14
-9	1.255771E-01	1.614589E-14
-10	1.068126E-01	1.373327E-14
-11	1.030737E-01	1.325254E-14
-12	9.452182E-02	1.215301E-14
-13	8.929789E-02	1.148134E-14
-14	8.422303E-02	1.082885E-14
-15	8.075905E-02	1.038348E-14
-16	7.717162E-02	9.922232E-15
-17	7.497239E-02	9.639465E-15
-18	7.210869E-02	9.271270E-15
-19	7.092953E-02	9.119658E-15
-20	6.846428E-02	8.802695E-15

CALCULATED HALF-WIDTHS FOR HC43 PERTURBED BY HC-0 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 9.236362 BE(F) = 9.534647 BE(P) = 10.440470
MU(HC43) = 1.208E-18 MU(HC-0) = 1.108E-18
Q(HC43) = 7.600E-26 Q(HC-0) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.494796E-01	1.921911E-14
-2	1.853735E-01	2.383413E-14
-3	2.206487E-01	2.836958E-14
-4	2.043905E-01	2.627920E-14
-5	1.401108E-01	1.801454E-14
-6	1.551008E-01	1.994186E-14
-7	1.556926E-01	2.001794E-14
-8	1.218726E-01	1.566959E-14
-9	1.229590E-01	1.580927E-14
-10	1.141379E-01	1.467512E-14
-11	1.037613E-01	1.334096E-14
-12	9.804404E-02	1.260587E-14
-13	9.079379E-02	1.167368E-14
-14	8.556712E-02	1.100167E-14
-15	8.378667E-02	1.077275E-14
-16	7.860649E-02	1.010672E-14
-17	7.483113E-02	9.621305E-15
-18	7.381898E-02	9.491167E-15
-19	7.184279E-02	9.237081E-15
-20	7.043844E-02	9.056520E-15

CALCULATED HALF-WIDTHS FOR HC54 PERTURBED BY HC-0 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

```
BE(I) =  8.938384 BE(F) =  9.236362 BE(P) = 10.440470
MU(HC54) =     1.233E-18 MU(HC-0) =     1.108E-18
Q(HC54) =     7.600E-26 Q(HC-0) =     7.600E-26
B(MIN) =     3.100E-08
```

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.436180E-01	1.846548E-14
-2	1.659064E-01	2.133116E-14
-3	2.049376E-01	2.634954E-14
-4	2.000004E-01	2.571475E-14
-5	1.654608E-01	2.127388E-14
-6	1.835695E-01	2.360474E-14
-7	1.799455E-01	2.313622E-14
-8	1.474330E-01	1.895598E-14
-9	1.020102E-01	1.311581E-14
-10	9.511358E-02	1.222909E-14
-11	1.027514E-01	1.321112E-14
-12	9.999084E-02	1.285618E-14
-13	9.029698E-02	1.160980E-14
-14	8.864051E-02	1.139682E-14
-15	8.141094E-02	1.046729E-14
-16	7.720417E-02	9.926416E-15
-17	7.753527E-02	9.968981E-15
-18	7.571805E-02	9.735339E-15
-19	7.219434E-02	9.282282E-15
-20	6.722885E-02	8.643853E-15

CALCULATED HALF-WIDTHS FOR HC65 PERTURBED BY HC-0 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

```
BE(I) =  8.638970 BE(F) =  8.938384 BE(P) = 10.440470
MU(HC65) =     1.256E-18 MU(HC-0) =     1.108E-18
Q(HC65) =     7.600E-26 Q(HC-0) =     7.600E-26
B(MIN) =     3.100E-08
```

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.586179E-01	2.039405E-14
-2	1.538802E-01	1.978492E-14
-3	1.921510E-01	2.470553E-14
-4	1.492031E-01	1.918357E-14
-5	1.925095E-01	2.475163E-14
-6	1.759033E-01	2.261650E-14
-7	1.858521E-01	2.389565E-14
-8	1.609110E-01	2.068889E-14
-9	1.423728E-01	1.830537E-14
-10	1.252192E-01	1.609988E-14
-11	1.074846E-01	1.381967E-14
-12	1.015506E-01	1.305672E-14
-13	9.769571E-02	1.256108E-14
-14	9.099823E-02	1.169996E-14
-15	8.285493E-02	1.065295E-14
-16	7.718980E-02	9.924570E-15
-17	7.893491E-02	1.014894E-14
-18	7.729506E-02	9.938102E-15
-19	7.489496E-02	9.629508E-15
-20	6.757474E-02	8.688322E-15

CALCULATED HALF-WIDTHS FOR HC76 PERTURBED BY HC-O AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 8.335323 BE(P) = 8.638970 BE(P) = 10.440470
MU(HC76) = 1.276E-18 MU(HC-O) = 1.108E-18
Q(HC76) = 7.600E-26 Q(HC-O) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	2.028314E-01	2.607875E-14
-2	1.559864E-01	2.005572E-14
-3	1.945512E-01	2.501412E-14
-4	1.749976E-01	2.250006E-14
-5	1.704365E-01	2.191362E-14
-6	1.808475E-01	2.325220E-14
-7	9.016705E-02	1.159309E-14
-8	1.522762E-01	1.957869E-14
-9	9.743136E-02	1.252709E-14
-10	1.199182E-01	1.541830E-14
-11	1.048989E-01	1.348721E-14
-12	1.060706E-01	1.363787E-14
-13	9.267890E-02	1.191606E-14
-14	9.091938E-02	1.168983E-14
-15	8.777362E-02	1.128536E-14
-16	8.586985E-02	1.104059E-14
-17	8.246523E-02	1.060284E-14
-18	7.535946E-02	9.689234E-15
-19	6.975865E-02	8.969117E-15
-20	7.328403E-02	9.422388E-15

CALCULATED HALF-WIDTHS FOR HC37 [BROADENED] BY HC-0 AT [300.0] DEG. K

INPUT CONSTANTS ARE:

BE(I) = 8.026087 BE(F) = 8.335823 BE(P) = 10.440470
MU(HC37) = 1.292E-18 MU(HC-0) = 1.108E-18
Q(HC37) = 7.600E-26 Q(HC-0) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.981196E-01	2.547293E-14
-2	1.716451E-01	2.206901E-14
-3	1.331509E-01	1.711968E-14
-4	1.822292E-01	2.342985E-14
-5	1.850726E-01	2.379544E-14
-6	1.231090E-01	1.582856E-14
-7	1.711808E-01	2.200931E-14
-8	1.424549E-01	1.831593E-14
-9	1.151838E-01	1.480959E-14
-10	1.318772E-01	1.695592E-14
-11	1.048993E-01	1.348728E-14
-12	9.967643E-02	1.281575E-14
-13	9.960467E-02	1.280652E-14
-14	9.828556E-02	1.263692E-14
-15	9.197748E-02	1.182587E-14
-16	8.455044E-02	1.087095E-14
-17	7.457495E-02	9.588362E-15
-18	8.014309E-02	1.030428E-14
-19	7.803613E-02	1.003338E-14
-20	7.645261E-02	9.829787E-15

CALCULATED HALF-WIDTHS FOR HC33 PERTURBED BY HC-O AT 300.0 DEG. K

INPUT CONSTANTS ARE:

```
BE(I) =   7.7[illegible]357 BE(F) =  8.026087 BE(P) = 10.440470
MU(HC33) =      1.304E-18 MU(HC-O) =      1.108E-18
Q(HC33) =      7.600E-26 Q(HC-O) =      7.600E-26
B(MIN) =      3.100E-08
```

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.822262E-01	2.342946E-14
-2	1.537125E-01	1.976335E-14
-3	1.342102E-01	1.725587E-14
-4	1.203650E-01	1.547575E-14
-5	1.626888E-01	2.091747E-14
-6	2.153939E-01	2.769395E-14
-7	1.739804E-01	2.236927E-14
-8	1.477669E-01	1.899891E-14
-9	1.649750E-01	2.121142E-14
-10	1.356633E-01	1.744271E-14
-11	1.293707E-01	1.663365E-14
-12	1.196221E-01	1.538024E-14
-13	1.056159E-01	1.357940E-14
-14	9.660912E-02	1.242138E-14
-15	9.156656E-02	1.177303E-14
-16	8.944958E-02	1.150085E-14
-17	8.257622E-02	1.061711E-14
-18	8.366680E-02	1.075734E-14
-19	7.844126E-02	1.008547E-14
-20	7.840902E-02	1.008133E-14

CALCULATED HALF-WIDTHS FOR HCO9 PERTURBED BY HC-O AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 7.372670 BE(F) = 7.706357 BE(P) = 10.440470
MU(HC09) = 1.306E-18 MU(HC-0) = 1.108E-18
Q(HC09) = 7.600E-26 Q(HC-0) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.913689E-01	2.460497E-14
-2	9.508646E-02	1.222560E-14
-3	2.179596E-01	2.802383E-14
-4	2.590963E-01	3.331291E-14
-5	1.526800E-01	1.963061E-14
-6	1.577269E-01	2.027950E-14
-7	1.592501E-01	2.047534E-14
-8	1.705241E-01	2.192438E-14
-9	1.607572E-01	2.066912E-14
-10	1.490168E-01	1.915961E-14
-11	1.358721E-01	1.746956E-14
-12	1.125532E-01	1.447136E-14
-13	1.005304E-01	1.292556E-14
-14	1.027955E-01	1.321678E-14
-15	9.862041E-02	1.267997E-14
-16	9.276420E-02	1.192702E-14
-17	7.991558E-02	1.027503E-14
-18	8.673763E-02	1.115216E-14
-19	8.360153E-02	1.074895E-14
-20	7.565188E-02	9.726832E-15

CALCULATED HALF-WIDTHS FOR HC10 PERTURBED BY HC-1 AT [illegible] DEG. K

INPUT CONSTANTS ARE:

```
BE(I) = 10.136340 BE(F) = 10.440470 BE(P) = 10.136340
MU(HC10) =     1.123E-18 MU(HC-1) =     1.138E-18
Q(HC10) =     7.600E-26 Q(HC-1) =     7.600E-26
B(MIN) =     3.100E-08
```

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	2.182547E-01	2.806176E-14
-2	2.473986E-01	3.180893E-14
-3	2.688269E-01	3.456402E-14
-4	2.657143E-01	3.416383E-14
-5	2.395893E-01	3.080484E-14
-6	2.017947E-01	2.594545E-14
-7	1.666402E-01	2.142551E-14
-8	1.395760E-01	1.794577E-14
-9	1.182643E-01	1.520572E-14
-10	1.055292E-01	1.356827E-14
-11	9.526235E-02	1.224822E-14
-12	8.949512E-02	1.150671E-14
-13	8.389503E-02	1.078668E-14
-14	8.065504E-02	1.037010E-14
-15	7.684213E-02	9.879863E-15
-16	7.452965E-02	9.582541E-15
-17	7.200223E-02	9.257579E-15
-18	7.038701E-02	9.049910E-15
-19	6.889778E-02	8.858433E-15
-20	6.791210E-02	8.731704E-15

CALCULATED HALF-WIDTHS FOR HC21 PERTURBED BY HC-1 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 9.834431 BE(P) = 10.136340 BE(P) = 10.136340
MU(HC21) = 1.152E-18 MU(HC-1) = 1.138E-18
Q(HC21) = 7.600E-26 Q(HC-1) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	9.583396E-02	1.232171E-14
-2	1.167887E-01	1.501593E-14
-3	1.602815E-01	2.060796E-14
-4	2.562184E-01	3.294290E-14
-5	1.506556E-01	1.937033E-14
-6	1.489395E-01	1.914968E-14
-7	1.231339E-01	1.583176E-14
-8	1.288126E-01	1.656188E-14
-9	7.482284E-02	9.620234E-15
-10	9.206963E-02	1.183772E-14
-11	8.302951E-02	1.067540E-14
-12	7.558644E-02	9.718416E-15
-13	7.551831E-02	9.709654E-15
-14	7.473803E-02	9.609335E-15
-15	6.942677E-02	8.926447E-15
-16	6.866956E-02	8.829092E-15
-17	6.493050E-02	8.348347E-15
-18	6.110377E-02	7.856325E-15
-19	6.190945E-02	7.959914E-15
-20	6.145886E-02	7.901981E-15

CALCULATED HALF-WIDTHS FOR HC32 PERTURBED BY HC-1 AT 300.0 DEG. K
INPUT CONSTANTS ARE:
BE(I) = 9.534647 BE(F) = 9.834431 BE(P) = 10.136340
MU(HC32) = 1.181E-18 MU(HC-1) = 1.138E-18
Q(HC32) = 7.600E-26 Q(HC-1) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	2.292388E-01	2.947404E-14
-2	2.563255E-01	3.295667E-14
-3	2.695206E-01	3.465321E-14
-4	2.587906E-01	3.327361E-14
-5	2.320123E-01	2.983064E-14
-6	1.943647E-01	2.499015E-14
-7	1.659985E-01	2.134301E-14
-8	1.408136E-01	1.810490E-14
-9	1.249192E-01	1.606130E-14
-10	1.120100E-01	1.440152E-14
-11	1.019485E-01	1.310788E-14
-12	9.588557E-02	1.232834E-14
-13	8.878195E-02	1.141501E-14
-14	8.504486E-02	1.093452E-14
-15	8.042383E-02	1.034037E-14
-16	7.745498E-02	9.958658E-15
-17	7.466805E-02	9.600339E-15
-18	7.239527E-02	9.308113E-15
-19	7.077980E-02	9.100407E-15
-20	6.922984E-02	8.901124E-15

```
 CALCULATED HALF-WIDTHS FOR HC43 PERTURBED BY HC-1 AT  300.0 DEG. K
INPUT CONSTANTS ARE:
BE(I) =  9.236362 BE(F) =  9.534647 BE(P) = 10.136340
MU(HC43) =      1.208E-18 MU(HC-1) =      1.138E-18
Q(HC43) =      7.600E-26 Q(HC-1) =      7.600E-26
B(MIN) =     3.100E-08
```

LINE N	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.130792E-01	1.453899E-14
-2	2.045076E-01	2.629428E-14
-3	1.915412E-01	2.462712E-14
-4	2.167128E-01	2.786353E-14
-5	1.854725E-01	2.364686E-14
-6	1.705298E-01	2.192562E-14
-7	1.596113E-01	2.052178E-14
-8	1.203172E-01	1.546961E-14
-9	1.313053E-01	1.688239E-14
-10	1.093220E-01	1.405591E-14
-11	9.859508E-02	1.267672E-14
-12	8.563226E-02	1.101004E-14
-13	8.342648E-02	1.072644E-14
-14	7.594252E-02	9.764199E-15
-15	7.527083E-02	9.677839E-15
-16	7.148826E-02	9.191500E-15
-17	6.922591E-02	8.900619E-15
-18	6.513339E-02	8.374435E-15
-19	6.153741E-02	7.912081E-15
-20	6.264126E-02	8.054006E-15

INPUT CONSTANTS ARE:
BE(I) = 8.938384 BE(P) = 9.236362 BE(P) = 10.136340
MU(HC54) = 1.233E-18 MU(HC-1) = 1.133E-18
Q(HC54) = 7.600E-26 Q(HC-1) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.530634E-01	1.967990E-14
-2	2.043236E-01	2.627060E-14
-3	2.264403E-01	2.911422E-14
-4	2.115138E-01	2.719507E-14
-5	1.806495E-01	2.322674E-14
-6	1.911325E-01	2.457457E-14
-7	1.803609E-01	2.326935E-14
-8	1.282027E-01	1.648347E-14
-9	1.204098E-01	1.548152E-14
-10	1.189107E-01	1.528877E-14
-11	9.966767E-02	1.281462E-14
-12	8.673441E-02	1.115175E-14
-13	7.953221E-02	1.022574E-14
-14	8.045918E-02	1.034492E-14
-15	7.490051E-02	9.630223E-15
-16	7.306194E-02	9.393333E-15
-17	6.895453E-02	8.865724E-15
-18	6.363833E-02	8.182203E-15
-19	6.586415E-02	8.468388E-15
-20	6.437266E-02	8.276620E-15

CALCULATED HALF-WIDTHS FOR HC65 PERTURBED BY HC-1 AT 300.0 DEG. K
INPUT CONSTANTS ARE:
BE(I) = 8.638970 BE(F) = 8.933384 BE(P) = 10.136340
MU(HC65) = 1.256E-18 MU(HC-1) = 1.133E-18
Q(HC65) = 7.600E-26 Q(HC-1) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.486462E-01	1.388153E-14
-2	1.694433E-01	2.178599E-14
-3	1.868303E-01	2.402143E-14
-4	2.119517E-01	2.725137E-14
-5	2.199011E-01	2.827346E-14
-6	1.785766E-01	2.296022E-14
-7	1.595453E-01	2.051330E-14
-8	1.792657E-01	2.305139E-14
-9	1.048453E-01	1.343034E-14
-10	1.132179E-01	1.455633E-14
-11	9.784406E-02	1.258015E-14
-12	9.533262E-02	1.225725E-14
-13	8.536321E-02	1.097545E-14
-14	7.542628E-02	9.697823E-15
-15	7.043964E-02	9.056676E-15
-16	7.566923E-02	9.729064E-15
-17	6.995618E-02	8.994518E-15
-18	6.510967E-02	8.371379E-15
-19	6.630629E-02	8.525234E-15
-20	6.439066E-02	8.278937E-15

MU(HC76) = 1.276E-18 MU(HC-1) = 1.136E-18
Q(HC76) = 7.600E-26 Q(HC-1) = 7.600E-26
B(MIN) = 3.100E-08

LINE	HALF-WIDTH	CROSS-SECTION
M	CM-1	CM**2
-1	1.613432E-01	2.082161E-14
-2	1.571208E-01	2.020158E-14
-3	1.442036E-01	1.854154E-14
-4	1.568150E-01	2.041941E-14
-5	1.200648E-01	1.543715E-14
-6	1.698029E-01	2.183216E-14
-7	1.031162E-01	1.325801E-14
-8	1.214401E-01	1.561397E-14
-9	1.482303E-01	1.905848E-14
-10	1.310365E-01	1.684783E-14
-11	1.072319E-01	1.378713E-14
-12	9.479171E-02	1.218771E-14
-13	7.983756E-02	1.026500E-14
-14	8.526820E-02	1.096323E-14
-15	7.351774E-02	9.452437E-15
-16	7.531536E-02	9.683565E-15
-17	7.376331E-02	9.484008E-15
-18	7.187450E-02	9.241160E-15
-19	6.940436E-02	8.923563E-15
-20	6.514561E-02	8.376004E-15

```
CALCULATED HALF-WIDTHS FOR HC87 PERTURBED BY HC-1 AT  300.0 DEG. K
INPUT CONSTANTS ARE:
BE(I) =  8.026087 BE(F) =  8.335823 BE(P) = 10.136340
MU(HC87) =      1.292E-18 MU(HC-1) =      1.138E-18
Q(HC87) =     7.600E-26 Q(HC-1) =      7.600E-26
B(MIN) =     3.100E-08
```

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	2.066449E-01	2.656906E-14
-2	1.758620E-01	2.293262E-14
-3	2.030343E-01	2.610484E-14
-4	1.796993E-01	2.310457E-14
-5	1.208714E-01	1.554086E-14
-6	1.643459E-01	2.113052E-14
-7	1.123984E-01	1.445145E-14
-8	1.716732E-01	2.207263E-14
-9	1.144933E-01	1.472098E-14
-10	1.091713E-01	1.403655E-14
-11	1.025671E-01	1.318741E-14
-12	9.980055E-02	1.283942E-14
-13	8.838946E-02	1.136454E-14
-14	8.611089E-02	1.107158E-14
-15	7.720381E-02	9.926366E-15
-16	8.018416E-02	1.030956E-14
-17	7.726240E-02	9.933901E-15
-18	7.145452E-02	9.187163E-15
-19	6.896818E-02	8.867486E-15
-20	6.794387E-02	8.735786E-15

CALCULATED HALF-WIDTHS FOR HC98 PERTURBED BY HC-1 AT 300.0 DEG. K
INPUT CONSTANTS ARE:
BE(I) = 7.706357 BE(F) = 8.026087 BE(P) = 10.136340
MU(HC98) = 1.304E-18 MU(HC-1) = 1.138E-18
Q(HC98) = 7.600E-26 Q(HC-1) = 7.600E-26

B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	2.017953E-01	2.594554E-14
-2	1.546862E-01	1.988854E-14
-3	1.393250E-01	1.791351E-14
-4	1.876442E-01	2.415178E-14
-5	1.872874E-01	2.403021E-14
-6	1.347713E-01	1.732803E-14
-7	2.002630E-01	2.574851E-14
-8	1.713045E-01	2.202522E-14
-9	1.644711E-01	2.114562E-14
-10	1.361741E-01	1.750838E-14
-11	1.275268E-01	1.639657E-14
-12	1.126135E-01	1.447912E-14
-13	9.577656E-02	1.231433E-14
-14	9.083909E-02	1.167950E-14
-15	8.745521E-02	1.124442E-14
-16	8.087301E-02	1.039813E-14
-17	7.954156E-02	1.022694E-14
-18	6.804860E-02	8.749247E-15
-19	7.001293E-02	9.001609E-15
-20	7.042658E-02	9.054996E-15

CALCULATED HALF-WIDTHS FOR HC09 PERTURBED BY HC-1 AT 300.0 DEG. K
INPUT CONSTANTS ARE:
BE(I) = 7.372670 BE(F) = 7.706357 BE(P) = 10.136340
MU(HC09) = 1.308E-18 MU(HC-1) = 1.138E-18
Q(HC09) = 7.600E-26 Q(HC-1) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.978576E-01	2.543925E-14
-2	1.583527E-01	2.035996E-14
-3	1.421350E-01	1.827480E-14
-4	1.131353E-01	1.454621E-14
-5	1.576465E-01	2.026917E-14
-6	2.275953E-01	2.926273E-14
-7	2.153500E-01	2.768830E-14
-8	1.538376E-01	1.977944E-14
-9	1.231748E-01	1.583702E-14
-10	1.465935E-01	1.884868E-14
-11	1.192189E-01	1.532839E-14
-12	1.185951E-01	1.524819E-14
-13	1.102273E-01	1.417232E-14
-14	9.274715E-02	1.192483E-14
-15	9.245145E-02	1.188681E-14
-16	8.484888E-02	1.090932E-14
-17	7.472724E-02	9.607946E-15
-18	7.091445E-02	9.117720E-15
-19	7.400692E-02	9.515328E-15
-20	6.533713E-02	8.407056E-15

CALCULATED HALF-WIDTHS FOR HC10 PERTURBED BY HC-2 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 10.136340 BE(F) = 10.440470 BE(P) = 9.834431
MU(HC10) = 1.123E-18 MU(HC-2) = 1.167E-18
Q(HC10) = 7.600E-26 Q(HC-2) = 7.600E-26
B(MIN) = 3.100E-08

LINE N	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	2.264956E-01	2.912134E-14
-2	2.558067E-01	3.288997E-14
-3	2.710969E-01	3.485588E-14
-4	2.588442E-01	3.328050E-14
-5	2.249005E-01	2.891624E-14
-6	1.868770E-01	2.402743E-14
-7	1.541384E-01	1.981812E-14
-8	1.327473E-01	1.706779E-14
-9	1.153227E-01	1.482745E-14
-10	1.046887E-01	1.346020E-14
-11	9.648120E-02	1.240493E-14
-12	8.966362E-02	1.152837E-14
-13	8.508873E-02	1.094016E-14
-14	8.038294E-02	1.033512E-14
-15	7.724285E-02	9.931387E-15
-16	7.414895E-02	9.533596E-15
-17	7.207078E-02	9.266395E-15
-18	7.023054E-02	9.029788E-15
-19	6.907630E-02	8.881384E-15
-20	6.799507E-02	8.742369E-15

CALCULATED HALF-WIDTHS FOR HC21 PERTURBED BY HC-2 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

```
BE(I) =   9.834431 BE(F) = 10.136340 BE(P) =   9.834431
MU(HC21) =      1.152E-18 MU(HC-2) =      1.167E-18
Q(HC21) =     7.600E-26 Q(HC-2) =     7.600E-26
B(MIN) =     3.100E-08
```

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.014140E-01	1.303916E-14
-2	5.087056E-02	6.540605E-15
-3	1.561040E-01	2.007085E-14
-4	1.508378E-01	1.939374E-14
-5	2.339771E-01	3.008326E-14
-6	1.955163E-01	2.513822E-14
-7	1.471796E-01	1.892340E-14
-8	1.101904E-01	1.416756E-14
-9	1.161537E-01	1.493429E-14
-10	9.721394E-02	1.249991E-14
-11	8.588213E-02	1.104217E-14
-12	8.351582E-02	1.073793E-14
-13	7.535362E-02	9.688485E-15
-14	7.464260E-02	9.597063E-15
-15	6.919199E-02	8.896262E-15
-16	6.843150E-02	8.798477E-15
-17	6.490839E-02	8.345504E-15
-18	6.413651E-02	8.246255E-15
-19	6.211030E-02	7.985739E-15
-20	6.148313E-02	7.905101E-15

CALCULATED HALF-WIDTHS FOR HC32 PERTURBED BY HC-2 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

```
BE(I) =  9.534647 BE(F) =  9.834431 BE(P) =  9.834431
MU(HC32) =      1.161E-18 MU(HC-2) =      1.167E-18
Q(HC32) =     7.600E-26 Q(HC-2) =     7.600E-26
B(MIN) =     3.100E-08
```

LINE N	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.023274E-01	1.315660E-14
-2	1.001570E-01	1.287754E-14
-3	1.028388E-01	1.322235E-14
-4	2.034703E-01	2.616089E-14
-5	1.321318E-01	1.698865E-14
-6	1.557797E-01	2.002914E-14
-7	1.707931E-01	2.195946E-14
-8	1.343678E-01	1.727613E-14
-9	1.142910E-01	1.469480E-14
-10	9.117502E-02	1.172270E-14
-11	8.728474E-02	1.122251E-14
-12	7.613045E-02	9.788364E-15
-13	7.121629E-02	9.156531E-15
-14	7.020658E-02	9.026712E-15
-15	6.512767E-02	8.373697E-15
-16	6.511229E-02	8.371721E-15
-17	6.164388E-02	7.925769E-15
-18	6.203718E-02	7.976336E-15
-19	6.281424E-02	8.076246E-15
-20	6.030226E-02	7.753272E-15

CALCULATED HALF-WIDTHS FOR HC43 PERTURBED BY HC-2 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

```
BE(I) =  9.236362 BE(F) =  9.534647 BE(P) =  9.834431
MU(HC43) =     1.208E-18 MU(HC-2) =     1.167E-18
Q(HC43) =     7.600E-26 Q(HC-2) =     7.600E-26
E(MIN) =     3.100E-28
```

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.046873E-01	1.346002E-14
-2	1.014261E-01	1.304071E-14
-3	1.586236E-01	2.039480E-14
-4	1.941749E-01	2.496576E-14
-5	1.498582E-01	1.926779E-14
-6	1.437386E-01	1.848097E-14
-7	1.713790E-01	2.203479E-14
-8	1.295586E-01	1.665780E-14
-9	1.136420E-01	1.461135E-14
-10	1.082243E-01	1.391478E-14
-11	9.710109E-02	1.248463E-14
-12	8.971882E-02	1.153546E-14
-13	8.371425E-02	1.076343E-14
-14	7.968831E-02	1.024581E-14
-15	7.447392E-02	9.575379E-15
-16	6.965631E-02	8.955957E-15
-17	6.887168E-02	8.855079E-15
-18	6.645054E-02	8.543784E-15
-19	6.472468E-02	8.321882E-15
-20	6.301671E-02	8.102280E-15

CALCULATED HALF-WIDTHS FOR HC54 PERTURBED BY HC-2 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 8.938384 BE(F) = 9.236362 BE(P) = 9.834431
MU(HC54) = 1.233E-18 MU(HC-2) = 1.167E-13
Q(HC54) = 7.600E-26 Q(HC-2) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.233819E-01	1.586365E-14
-2	1.435020E-01	1.845056E-14
-3	1.966070E-01	2.527845E-14
-4	2.223845E-01	2.859279E-14
-5	1.928644E-01	2.479726E-14
-6	1.867262E-01	2.400804E-14
-7	1.529523E-01	1.966561E-14
-8	1.361198E-01	1.750141E-14
-9	1.376454E-01	1.769755E-14
-10	9.889501E-02	1.271528E-14
-11	1.021156E-01	1.312936E-14
-12	8.622366E-02	1.108608E-14
-13	8.583277E-02	1.103583E-14
-14	8.074856E-02	1.038213E-14
-15	7.213801E-02	9.275038E-15
-16	7.118952E-02	9.153089E-15
-17	6.568122E-02	8.444863E-15
-18	6.742364E-02	8.668898E-15
-19	6.246281E-02	8.031062E-15
-20	6.367821E-02	8.187332E-15

CALCULATED HALF-WIDTHS FOR HC65 PERTURBED BY HC-2 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

```
BE(I) =   8.638970 BE(F) =   8.938384 BE(P) =   9.834431
MU(HC65) =      1.256E-18 MU(HC-2) =      1.167E-18
Q(HC65) =    .7.600E-26 Q(HC-2) =     7.600E-26
B(MIN) =     3.100E-08
```

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.779661E-01	2.288172E-14
-2	2.086460E-01	2.682635E-14
-3	2.292202E-01	2.947164E-14
-4	2.186685E-01	2.811497E-14
-5	1.906593E-01	2.451373E-14
-6	1.782153E-01	2.291377E-14
-7	1.598037E-01	2.054652E-14
-8	1.346825E-01	1.731661E-14
-9	1.175925E-01	1.511928E-14
-10	1.125472E-01	1.447059E-14
-11	9.321660E-02	1.198519E-14
-12	9.687084E-02	1.245502E-14
-13	8.103591E-02	1.041907E-14
-14	8.306837E-02	1.068040E-14
-15	8.019423E-02	1.031086E-14
-16	7.492286E-02	9.633096E-15
-17	7.242709E-02	9.312209E-15
-18	6.970096E-02	8.961700E-15
-19	6.233537E-02	8.014677E-15
-20	6.559843E-02	8.434226E-15

CALCULATED HALF-WIDTHS FOR HC76 PERTURBED BY HC-2 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 8.335823 BE(F) = 8.638970 BE(P) = 9.834431
MU(HC76) = 1.276E-18 MU(HC-2) = 1.167E-18
Q(HC76) = 7.600E-26 Q(HC-2) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.716664E-01	2.207176E-14
-2	1.723380E-01	2.215810E-14
-3	2.073951E-01	2.666552E-14
-4	2.189878E-01	2.815602E-14
-5	1.711144E-01	2.200076E-14
-6	1.252910E-01	1.610911E-14
-7	1.643074E-01	2.112557E-14
-8	1.599634E-01	2.056770E-14
-9	1.053362E-01	1.354345E-14
-10	1.341244E-01	1.724484E-14
-11	1.112980E-01	1.430997E-14
-12	9.969342E-02	1.281793E-14
-13	8.806419E-02	1.132272E-14
-14	8.571911E-02	1.102121E-14
-15	8.147907E-02	1.047606E-14
-16	7.817298E-02	1.005098E-14
-17	7.126522E-02	9.162820E-15
-18	6.635427E-02	8.531407E-15
-19	6.778294E-02	8.715092E-15
-20	6.670272E-02	8.576205E-15

CALCULATED HALF-WIDTHS FOR HC37 PERTURBED BY HC-2 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 8.026087 BE(F) = 8.335823 BE(P) = 9.834431
MU(HC37) = 1.292E-18 MU(HC-2) = 1.167E-18
Q(HC37) = 7.600E-26 Q(HC-2) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.649155E-01	2.120376E-14
-2	1.561027E-01	2.007068E-14
-3	1.998097E-01	2.569023E-14
-4	1.668735E-01	2.145551E-14
-5	1.880376E-01	2.417665E-14
-6	1.987184E-01	2.554993E-14
-7	1.351502E-01	1.737674E-14
-8	1.817688E-01	2.337066E-14
-9	1.550012E-01	1.992906E-14
-10	1.379393E-01	1.773535E-14
-11	1.146486E-01	1.474078E-14
-12	1.133290E-01	1.457110E-14
-13	7.684410E-02	9.880118E-15
-14	8.239663E-02	1.059403E-14
-15	8.126813E-02	1.044893E-14
-16	7.712293E-02	9.915964E-15
-17	7.609314E-02	9.783566E-15
-18	7.350165E-02	9.450367E-15
-19	7.120407E-02	9.154962E-15
-20	6.615889E-02	8.506284E-15

CALCULATED HALF-WIDTHS FOR HC98 PERTURBED BY HC-2 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 7.706357 BE(F) = 8.026087 BE(P) = 9.834431
MU(HC98) = 1.304E-18 MU(HC-2) = 1.167E-18
Q(HC98) = 7.600E-26 Q(HC-2) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	2.098323E-01	2.693658E-14
-2	1.749697E-01	2.249647E-14
-3	2.119406E-01	2.724995E-14
-4	1.916666E-01	2.464325E-14
-5	1.230657E-01	1.582299E-14
-6	1.646376E-01	2.116804E-14
-7	2.056089E-01	2.643586E-14
-8	1.802047E-01	2.316955E-14
-9	1.404544E-01	1.805871E-14
-10	1.234382E-01	1.587088E-14
-11	1.066900E-01	1.371751E-14
-12	1.102434E-01	1.417439E-14
-13	9.886694E-02	1.271167E-14
-14	8.876443E-02	1.141276E-14
-15	8.629203E-02	1.109487E-14
-16	7.895029E-02	1.015092E-14
-17	7.246059E-02	9.316519E-15
-18	7.402539E-02	9.517709E-15
-19	7.103300E-02	9.132967E-15
-20	6.855124E-02	8.813879E-15

CALCULATED HALF-WIDTHS FOR HCOO PERTURBED BY HC-2 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 7.372670 BE(F) = 7.706357 BE(P) = 9.834431
MU(HCOO) = 1.308E-18 MU(HC-2) = 1.167E-18
Q(HCOO) = 7.600E-26 Q(HC-2) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	2.048370E-01	2.633661E-14
-2	1.619853E-01	2.082702E-14
-3	1.330367E-01	1.710499E-14
-4	1.353223E-01	1.739886E-14
-5	2.511989E-01	3.229752E-14
-6	2.313782E-01	2.974910E-14
-7	2.067174E-01	2.657833E-14
-8	1.926144E-01	2.476511E-14
-9	1.711951E-01	2.201115E-14
-10	1.556476E-01	2.001215E-14
-11	1.361690E-01	1.750772E-14
-12	1.108358E-01	1.425055E-14
-13	1.009411E-01	1.297835E-14
-14	8.811235E-02	1.132892E-14
-15	8.227211E-02	1.057802E-14
-16	7.709301E-02	9.912122E-15
-17	8.238608E-02	1.059267E-14
-18	7.889527E-02	1.014385E-14
-19	7.033420E-02	9.043117E-15
-20	6.643236E-02	8.541443E-15

CALCULATED HALF-WIDTHS FOR HC10 PERTURBED BY HC-3 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 10.136340 BE(F) = 10.440470 BE(P) = 9.534647
MU(HC10) = 1.123E-18 MU(HC-3) = 1.195E-18
Q(HC10) = 7.600E-26 Q(HC-3) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	2.307678E-01	2.967063E-14
-2	2.496798E-01	3.210221E-14
-3	2.503091E-01	3.218311E-14
-4	2.295738E-01	2.951711E-14
-5	1.968358E-01	2.530787E-14
-6	1.679928E-01	2.159942E-14
-7	1.444316E-01	1.857008E-14
-8	1.292578E-01	1.661913E-14
-9	1.149102E-01	1.477441E-14
-10	1.038596E-01	1.335360E-14
-11	9.433115E-02	1.212849E-14
-12	8.839935E-02	1.136582E-14
-13	8.340031E-02	1.072307E-14
-14	7.954383E-02	1.022724E-14
-15	7.695502E-02	9.894378E-15
-16	7.397026E-02	9.510615E-15
-17	7.213527E-02	9.274686E-15
-18	7.041138E-02	9.053044E-15
-19	6.910801E-02	8.885460E-15
-20	6.825918E-02	8.776322E-15

CALCULATED HALF-WIDTHS FOR HC21 PERTURBED BY HC-3 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

```
BE(I) =  9.834431 BE(P) = 10.136340 BE(P) =  9.534647
MU(HC21) =     1.152E-18 MU(HC-3) =     1.195E-18
Q(HC21) =     7.600E-26 Q(HC-3) =     7.600E-26
B(MIN) =    3.100E-08
```

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.057048E-01	1.359083E-14
-2	9.840292E-02	1.265201E-14
-3	2.171428E-01	2.791881E-14
-4	1.497781E-01	1.925750E-14
-5	2.309414E-01	2.969295E-14
-6	1.787698E-01	2.298507E-14
-7	1.421303E-01	1.827419E-14
-8	1.377743E-01	1.771412E-14
-9	1.110618E-01	1.428218E-14
-10	1.006500E-01	1.294093E-14
-11	9.195578E-02	1.182308E-14
-12	8.467442E-02	1.088689E-14
-13	7.972848E-02	1.025097E-14
-14	7.487988E-02	9.627573E-15
-15	7.126570E-02	9.162884E-15
-16	6.713635E-02	8.631957E-15
-17	6.255507E-02	8.042927E-15
-18	6.406146E-02	8.236609E-15
-19	6.073537E-02	7.808959E-15
-20	6.158427E-02	7.918105E-15

CALCULATED HALF-WIDTHS FOR HC32 PERTURBED BY HC-3 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 9.534647 BE(F) = 9.834431 BE(P) = 9.534647
MU(HC32) = 1.181E-18 MU(HC-3) = 1.195E-18
Q(HC32) = 7.600E-26 Q(HC-3) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.042287E-01	1.340105E-14
-2	5.257101E-02	6.759238E-15
-3	1.495970E-01	1.923421E-14
-4	1.703359E-01	2.190069E-14
-5	1.880555E-01	2.417895E-14
-6	1.686349E-01	2.168198E-14
-7	1.541578E-01	1.982060E-14
-8	1.232982E-01	1.585289E-14
-9	1.135527E-01	1.459988E-14
-10	1.047502E-01	1.346811E-14
-11	8.840817E-02	1.136695E-14
-12	8.569378E-02	1.101795E-14
-13	7.722420E-02	9.928988E-15
-14	7.694310E-02	9.892850E-15
-15	7.063609E-02	9.081931E-15
-16	7.003433E-02	9.004563E-15
-17	6.602198E-02	8.488680E-15
-18	6.526017E-02	8.390729E-15
-19	6.294781E-02	8.093427E-15
-20	6.226145E-02	8.005173E-15

CALCULATED HALF-WIDTHS FOR HC43 PERTURBED BY HC-3 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 9.236362 BE(F) = 9.534647 BE(P) = 9.534647
MU(HC43) = 1.208E-18 MU(HC-3) = 1.195E-18
Q(HC43) = 7.600E-26 Q(HC-3) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.212890E-01	1.559456E-14
-2	1.199617E-01	1.542390E-14
-3	1.071099E-01	1.377150E-14
-4	9.298605E-02	1.195554E-14
-5	1.349538E-01	1.735149E-14
-6	1.324773E-01	1.703307E-14
-7	1.022412E-01	1.314552E-14
-8	1.005192E-01	1.292412E-14
-9	9.538424E-02	1.226389E-14
-10	7.936388E-02	1.020409E-14
-11	8.471406E-02	1.089198E-14
-12	8.170718E-02	1.050538E-14
-13	7.997358E-02	1.028249E-14
-14	7.199967E-02	9.257250E-15
-15	7.241875E-02	9.311138E-15
-16	6.638175E-02	8.534934E-15
-17	6.729734E-02	8.652655E-15
-18	6.299400E-02	8.099363E-15
-19	6.374800E-02	8.196304E-15
-20	6.100529E-02	7.843664E-15

CALCULATED HALF-WIDTHS FOR HC54 PERTURBED BY HC-3 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 8.938384 BE(F) = 9.236362 BE(P) = 9.534647
MU(HC54) = 1.233E-18 MU(HC-3) = 1.195E-18
Q(HC54) = 7.600E-26 Q(HC-3) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	2.412975E-01	3.102447E-14
-2	2.706469E-01	3.479802E-14
-3	2.857183E-01	3.673581E-14
-4	2.763905E-01	3.553649E-14
-5	2.497953E-01	3.211706E-14
-6	2.111277E-01	2.714543E-14
-7	1.803469E-01	2.318784E-14
-8	1.529379E-01	1.966377E-14
-9	1.349409E-01	1.734983E-14
-10	1.201172E-01	1.544390E-14
-11	1.085010E-01	1.395036E-14
-12	1.010876E-01	1.299719E-14
-13	9.328359E-02	1.199380E-14
-14	8.871800E-02	1.140679E-14
-15	8.390218E-02	1.078760E-14
-16	8.043534E-02	1.034186E-14
-17	7.749659E-02	9.964011E-15
-18	7.484323E-02	9.622857E-15
-19	7.298553E-02	9.384010E-15
-20	7.111764E-02	9.143846E-15

CALCULATED HALF-WIDTHS FOR HC65 PERTURBED BY HC-3 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 8.638970 BE(F) = 8.938384 BE(P) = 9.534647
MU(HC65) = 1.256E-18 MU(HC-3) = 1.195E-18
Q(HC65) = 7.600E-26 Q(HC-3) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.267186E-01	1.629266E-14
-2	1.463550E-01	1.881738E-14
-3	2.015922E-01	2.591941E-14
-4	2.366118E-01	3.042200E-14
-5	1.994089E-01	2.563870E-14
-6	1.964489E-01	2.525813E-14
-7	1.757196E-01	2.259288E-14
-8	1.148951E-01	1.477247E-14
-9	1.445369E-01	1.858361E-14
-10	1.249183E-01	1.606118E-14
-11	1.016675E-01	1.307174E-14
-12	8.521789E-02	1.095676E-14
-13	8.714026E-02	1.120393E-14
-14	7.143337E-02	9.184443E-15
-15	7.270527E-02	9.347978E-15
-16	7.265532E-02	9.341550E-15
-17	6.681770E-02	8.590991E-15
-18	6.879067E-02	8.844660E-15
-19	6.715024E-02	8.633742E-15
-20	6.477964E-02	8.328950E-15

CALCULATED HALF-WIDTHS FOR HC76 PERTURBED BY HC-3 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 8.335823 BE(F) = 8.638970 BE(P) = 9.534647
MU(HC76) = 1.276E-18 MU(HC-3) = 1.195E-18
Q(HC76) = 7.600E-26 Q(HC-3) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.815105E-01	2.333744E-14
-2	2.120796E-01	2.726781E-14
-3	2.260234E-01	2.906062E-14
-4	2.225927E-01	2.861952E-14
-5	2.003007E-01	2.575337E-14
-6	2.192670E-01	2.819192E-14
-7	1.693166E-01	2.176963E-14
-8	1.197516E-01	1.539688E-14
-9	1.433131E-01	1.842627E-14
-10	1.235206E-01	1.588148E-14
-11	9.086698E-02	1.168309E-14
-12	1.003016E-01	1.289613E-14
-13	9.176010E-02	1.179792E-14
-14	8.147246E-02	1.047520E-14
-15	8.163357E-02	1.049591E-14
-16	7.712048E-02	9.915652E-15
-17	7.411957E-02	9.529819E-15
-18	7.146454E-02	9.188451E-15
-19	6.851387E-02	8.809068E-15
-20	6.684273E-02	8.594210E-15

CALCULATED HALF-WIDTHS FOR HC87 PERTURBED BY HC-3 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 8.026087 BE(P) = 8.335823 BE(P) = 9.534647
MU(HC87) = 1.292E-18 MU(HC-3) = 1.195E-18
Q(HC87) = 7.600E-26 Q(HC-3) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	1.745334E-01	2.244038E-14
-2	1.745487E-01	2.244233E-14
-3	2.115253E-01	2.719655E-14
-4	2.280044E-01	2.931533E-14
-5	2.007617E-01	2.581263E-14
-6	1.452291E-01	1.867261E-14
-7	2.124242E-01	2.731212E-14
-8	1.853359E-01	2.382929E-14
-9	1.589022E-01	2.043062E-14
-10	1.390032E-01	1.787213E-14
-11	1.236905E-01	1.590332E-14
-12	1.038538E-01	1.335285E-14
-13	9.097314E-02	1.169674E-14
-14	8.953810E-02	1.151223E-14
-15	8.005542E-02	1.029301E-14
-16	7.331824E-02	9.426789E-15
-17	7.498306E-02	9.640838E-15
-18	7.311481E-02	9.400629E-15
-19	6.971538E-02	8.963550E-15
-20	6.784314E-02	8.722833E-15

CALCULATED HALF-WIDTHS FOR HC98 PERTURBED BY HC-3 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 7.706357 BE(F) = 8.026087 BE(P) = 9.534647
MU(HC98) = 1.304E-18 MU(HC-3) = 1.195E-18
Q(HC98) = 7.600E-26 Q(HC-3) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	2.196474E-01	2.824083E-14
-2	1.544102E-01	1.985306E-14
-3	1.961798E-01	2.522352E-14
-4	1.757512E-01	2.259695E-14
-5	1.949167E-01	2.506113E-14
-6	1.898429E-01	2.440877E-14
-7	1.357660E-01	1.745591E-14
-8	1.633815E-01	2.100653E-14
-9	1.463269E-01	1.881376E-14
-10	1.455439E-01	1.871309E-14
-11	1.236562E-01	1.589890E-14
-12	1.060117E-01	1.363030E-14
-13	9.740901E-02	1.252422E-14
-14	8.401114E-02	1.080161E-14
-15	8.443749E-02	1.085642E-14
-16	7.935089E-02	1.020242E-14
-17	7.850480E-02	1.009364E-14
-18	7.499379E-02	9.642216E-15
-19	7.281631E-02	9.362252E-15
-20	6.716949E-02	8.636219E-15

CALCULATED HALF-WIDTHS FOR HC09 PERTURBED BY HC-3 AT 300.0 DEG. K

INPUT CONSTANTS ARE:

BE(I) = 7.372670 BE(F) = 7.706357 BE(P) = 9.534647
MU(HC09) = 1.308E-18 MU(HC-3) = 1.195E-18
Q(HC09) = 7.600E-26 Q(HC-3) = 7.600E-26
B(MIN) = 3.100E-08

LINE M	HALF-WIDTH CM-1	CROSS-SECTION CM**2
-1	2.124305E-01	2.731293E-14
-2	1.859790E-01	2.391198E-14
-3	1.445940E-01	1.859095E-14
-4	1.295903E-01	1.666188E-14
-5	1.279038E-01	1.644504E-14
-6	1.624191E-01	2.088279E-14
-7	2.129009E-01	2.737341E-14
-8	1.372969E-01	1.765275E-14
-9	1.476516E-01	1.898408E-14
-10	1.402785E-01	1.803610E-14
-11	1.242890E-01	1.598027E-14
-12	1.155732E-01	1.485965E-14
-13	1.032665E-01	1.327733E-14
-14	9.441653E-02	1.213972E-14
-15	8.204180E-02	1.054841E-14
-16	8.328277E-02	1.070796E-14
-17	7.358629E-02	9.461250E-15
-18	7.651263E-02	9.837502E-15
-19	7.530636E-02	9.682407E-15
-20	6.965727E-02	8.956079E-15

APPENDIX 2

LEAST-SQUARE FIT PARAMETERS FOR HCl LINEWIDTHS

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HC10          BY          HC-0        200.0
  8.20750E-02   1.18922E+00  -1.58161E-02  -7.24607E-02   1.88110E-01
  9.11270E-03  -8.69417E-01
HC21          BY          HC-0        200.0
  8.36489E-02   5.50084E+00  -2.78863E-01  -2.59301E-01   5.00610E-01
 -7.49403E-02  -4.55572E+00
HC32          BY          HC-0        200.0
  7.61203E-02   4.39938E-01  -1.14901E-02   1.32792E-02   1.28617E-01
 -3.14609E-03  -1.95647E-01
HC43          BY          HC-0        200.0
  7.61389E-02  -8.13214E-01   3.69709E-02   1.09826E-01  -5.59410E-02
  1.17647E-02   9.52872E-01
HC54          BY          HC-0        200.0
  8.54757E-02  -2.44590E+00   6.98513E-02   2.59706E-01  -2.63077E-01
  3.02608E-02   2.41580E+00
HC65          BY          HC-0        200.0
  4.47219E-02  -3.96131E+00   3.73638E-01   8.72833E-02  -4.93358E-01
  1.18371E-01   3.69823E+00
HC76          BY          HC-0        200.0
  4.54566E-02  -1.51897E+00   2.69380E-01  -6.68381E-02  -2.60640E-01
  8.04128E-02   1.55741E+00
HC87          BY          HC-0        200.0
  8.90417E-02   6.66238E+00  -3.31357E-01  -3.12450E-01   5.05881E-01
 -9.47543E-02  -5.57616E+00
HC98          BY          HC-0        200.0
  9.77757E-02   7.02942E+00  -4.05384E-01  -2.55004E-01   4.47262E-01
 -1.02404E-01  -5.82090E+00
HC09          BY          HC-0        200.0
  1.38406E-01   9.87815E+00  -7.93755E-01  -1.09102E-01   8.31437E-01
 -2.37619E-01  -8.45386E+00
HC10          BY          HC-1        200.0
  8.21744E-02   1.37356E+00  -2.18672E-02  -8.78718E-02   2.05770E-01
  9.39437E-03  -1.03168E+00
HC21          BY          HC-1        200.0
  6.02615E-02   1.93525E+00   3.58097E-02  -2.26462E-01   3.05941E-01
  1.33729E-02  -1.56854E+00
HC32          BY          HC-1        200.0
  6.85308E-02   1.07024E+00   1.90499E-02  -9.06843E-02   2.02965E-01
  7.93651E-03  -7.85268E-01
HC43          BY          HC-1        200.0
  6.45700E-02   5.05587E-01   7.29623E-02  -7.89800E-02   1.46191E-01
  8.72912E-03  -2.69854E-01
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HC54        BY       HC-1      200.0
  7.51003E-02   -4.99810E-01    5.45518E-02    5.99117E-02   -2.56504E-02
  1.23006E-02    6.74990E-01
HC65        BY       HC-1      200.0
  8.23536E-02   -2.30000E+00    1.09197E-01    1.79426E-01   -2.86343E-01
  5.43755E-02    2.31264E+00
HC76        BY       HC-1      200.0
  5.55343E-02   -3.64636E+00    3.31422E-01    8.46772E-02   -5.05111E-01
  1.17091E-01    3.48743E+00
HC87        BY       HC-1      200.0
  3.78675E-02   -2.62918E+00    4.05650E-01   -1.19818E-01   -4.00767E-01
  1.30223E-01    2.57951E+00
HC98        BY       HC-1      200.0
  9.78474E-02    7.51799E+00   -4.15468E-01   -2.90314E-01    5.68000E-01
 -1.22546E-01   -6.31216E+00
HC09        BY       HC-1      200.0
  8.96937E-02    5.04398E+00   -2.54132E-01   -1.78718E-01    3.20737E-01
 -6.95771E-02   -4.15089E+00
HC10        BY       HC-2      200.0
  8.38806E-02    1.41365E+00   -3.34964E-02   -7.65970E-02    2.32704E-01
 -2.31024E-03   -1.06534E+00
HC21        BY       HC-2      200.0
  8.70161E-02    3.16544E+00   -1.22231E-01   -1.80879E-01    4.38247E-01
 -3.19565E-02   -2.66430E+00
HC32        BY       HC-2      200.0
  7.07607E-02    2.16700E+00    2.43779E-02   -2.33835E-01    3.16081E-01
  1.06769E-02   -1.76441E+00
HC43        BY       HC-2      200.0
  8.97669E-02    3.19162E+00   -1.41570E-01   -1.57135E-01    3.44058E-01
 -3.28612E-02   -2.55799E+00
HC54        BY       HC-2      200.0
  8.67969E-02    6.35936E-01   -1.14624E-02    1.17102E-03    1.52666E-01
 -8.53127E-03   -3.68568E-01
HC65        BY       HC-2      200.0
  1.03260E-01   -7.57667E-01   -5.41033E-02    2.05739E-01    2.93513E-02
 -7.57020E-03    7.39215E-01
HC76        BY       HC-2      200.0
  1.04788E-01   -2.51707E+00    2.53123E-02    2.93171E-01   -3.37550E-01
  4.45182E-02    2.54261E+00
HC87        BY       HC-2      200.0
  6.14926E-02   -4.02662E+00    3.51568E-01    1.00200E-01   -5.41743E-01
  1.25364E-01    3.86432E+00
HC98        BY       HC-2      200.0
  7.88679E-02    9.10064E-01    3.61757E-02   -9.63142E-02   -1.35432E-01
  4.13350E-02   -4.32588E-01
HC09        BY       HC-2      200.0
  7.75531E-02   -1.27198E+00    1.28975E-01    7.53629E-02   -3.15676E-01
  4.82797E-02    1.45241E+00
HC10        BY       HC-3      200.0
  8.80781E-02    9.46121E-01   -3.76007E-02   -1.91480E-02    1.65066E-01
 -8.92767E-03   -6.25003E-01
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HC21        BY        HC-3      200.0
  8.60739E-02   1.30634E+00  -3.52856E-02  -7.57409E-02   2.54302E-01
  5.08882E-04  -1.02503E+00
HC32        BY        HC-3      200.0
  8.05356E-02   1.93537E+00  -2.51241E-02  -1.51282E-01   2.82282E-01
  6.43881E-03  -1.54640E+00
HC43        BY        HC-3      200.0
  7.60850E-02   1.50503E+00   1.92908E-02  -1.43752E-01   2.19211E-01
  1.47049E-02  -1.12195E+00
HC54        BY        HC-3      200.0
  9.21440E-02   1.83172E+00  -8.02218E-02  -8.21555E-02   2.41796E-01
 -7.18594E-03  -1.38712E+00
HC65        BY        HC-3      200.0
  7.80078E-02  -1.70299E+00   1.46471E-01   9.66685E-02  -6.15764E-02
  3.45812E-02   1.67036E+00
HC76        BY        HC-3      200.0
  8.81079E-02  -6.57594E-01   3.28420E-02   1.00844E-01  -8.42777E-02
  1.70405E-02   8.54743E-01
HC87        BY        HC-3      200.0
  7.82585E-02  -2.25812E+00   1.69379E-01   1.44326E-01  -2.90668E-01
  5.27536E-02   2.27477E+00
HC98        BY        HC-3      200.0
  5.63583E-02  -2.69931E+00   3.49453E-01  -2.85751E-02  -3.62254E-01
  1.05601E-01   2.63630E+00
HC09        BY        HC-3      200.0
  8.73131E-02   1.48413E+00  -2.05824E-02  -7.74630E-02  -7.75042E-02
  2.00562E-02  -9.44862E-01
HC10        BY        HC-0      300.0
  6.33687E-02   2.39023E-01   2.09231E-02   3.85279E-03   1.95799E-02
  1.17422E-02  -9.01176E-02
HC21        BY        HC-0      300.0
  6.25398E-02  -1.74506E+00   1.18701E-01   1.17894E-01  -1.43376E-01
  2.95184E-02   1.50748E+00
HC32        BY        HC-0      300.0
  5.59229E-02  -4.16933E-01   1.03767E-01  -4.11339E-03   3.15926E-02
  1.58633E-02   3.01050E-01
HC43        BY        HC-0      300.0
  7.27931E-02   1.47210E+00  -7.14972E-02  -1.79249E-02   1.79828E-01
 -3.35694E-02  -1.28190E+00
HC54        BY        HC-0      300.0
  7.36656E-02   6.42471E-02  -1.01587E-02   6.07950E-02  -5.65700E-03
 -2.13064E-03  -4.45290E-03
HC65        BY        HC-0      300.0
  7.54380E-02   4.24456E-02  -2.45418E-02   1.09236E-01  -4.42814E-02
 -1.71201E-02   6.36592E-02
HC76        BY        HC-0      300.0
  5.83116E-02   1.26012E+00   4.76355E-02  -1.33362E-01   4.49495E-02
 -1.78371E-03  -9.42827E-01
HC87        BY        HC-0      300.0
  6.33325E-02  -2.13313E-02   8.32713E-02  -2.00633E-02  -8.38526E-02
  8.55152E-03   1.88982E-01
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HC98        BY       HC-0       300.0
   6.49040E-02   -1.91044E+00    1.62641E-01    1.35169E-01   -2.58872E-01
   2.28672E-02    1.81543E+00
HC09        BY       HC-0       300.0
   9.26454E-02    7.26205E+00   -3.93217E-01   -2.76739E-01    5.05136E-01
  -1.34474E-01   -6.12166E+00
HC10        BY       HC-1       300.0
   6.35986E-02    2.38581E-01    1.98932E-02    4.81012E-03    1.50646E-02
   1.32406E-02   -8.52965E-02
HC21        BY       HC-1       300.0
   5.93948E-02    2.33397E+00   -8.22282E-02   -1.33961E-01    1.61990E-01
  -1.90908E-02   -1.99336E+00
HC32        BY       HC-1       300.0
   6.25222E-02    3.26672E-01    3.36470E-02   -1.04618E-02    3.56950E-02
   8.96091E-03   -1.67019E-01
HC43        BY       HC-1       300.0
   5.16265E-02   -9.86646E-01    1.09275E-01    6.25893E-02   -2.85647E-02
   2.05511E-02    8.09068E-01
HC54        BY       HC-1       300.0
   6.47129E-02   -2.47202E-01    7.01425E-03    9.16871E-02    6.03127E-03
  -1.40183E-03    2.43335E-01
HC65        BY       HC-1       300.0
   6.13290E-02   -1.15244E-02    1.90709E-02    5.15156E-02   -5.37213E-02
   4.81767E-03    1.04195E-01
HC76        BY       HC-1       300.0
   5.89445E-02    7.34663E-01    1.22540E-02   -1.10116E-02    4.25742E-02
  -2.12974E-02   -5.53684E-01
HC87        BY       HC-1       300.0
   7.72924E-02    2.12833E+00   -1.38529E-01   -1.18029E-02    1.72174E-01
  -5.37120E-02   -1.71748E+00
HC98        BY       HC-1       300.0
   6.54956E-02    1.50046E+00   -4.71089E-02    1.92523E-03    1.36547E-02
  -4.07454E-02   -1.09755E+00
HC09        BY       HC-1       300.0
   5.29710E-02   -2.91504E+00    2.33282E-01    1.79493E-01   -3.62192E-01
   4.19308E-02    2.72121E+00
HC10        BY       HC-2       300.0
   6.20670E-02    4.94030E-01    1.85381E-02   -2.24954E-02    6.04716E-02
   7.86005E-03   -3.19268E-01
HC21        BY       HC-2       300.0
   5.37690E-02    4.95572E-01    3.18628E-02   -4.52295E-02   -1.31777E-01
   1.95886E-02   -2.71904E-01
HC32        BY       HC-2       300.0
   7.09780E-02    8.41899E-01   -1.05575E-01    7.77603E-02   -2.69260E-02
  -2.32237E-02   -6.14239E-01
HC43        BY       HC-2       300.0
   6.87033E-02    2.05587E+00   -1.17109E-01   -3.25516E-02    1.20974E-01
  -3.96320E-02   -1.72690E+00
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HC54        BY          HC-2        300.0
  6.07845E-02   1.26306E+00  -3.98051E-02  -2.65242E-02   6.78234E-02
 -1.49747E-02  -1.04219E+00
HC65        BY          HC-2        300.0
  6.11438E-02   3.02820E-01   1.93055E-02   1.18078E-02   3.85611E-02
 -3.97976E-04  -1.98693E-01
HC76        BY          HC-2        300.0
  6.60957E-02   2.72001E+00  -1.15352E-01  -8.89486E-02   2.27929E-01
 -5.28223E-02  -2.28884E+00
HC87        BY          HC-2        300.0
  7.14388E-02   1.23904E+00  -7.94309E-02   5.11896E-02   5.92529E-02
 -3.97921E-02  -9.70467E-01
HC98        BY          HC-2        300.0
  9.14902E-02   2.48447E+00  -2.40660E-01   8.88919E-02   1.79491E-01
 -8.29655E-02  -2.00066E+00
HC09        BY          HC-2        300.0
  5.39128E-02  -2.61803E+00   2.00500E-01   1.98960E-01  -4.04556E-01
  3.76474E-02   2.53206E+00
HC10        BY          HC-3        300.0
  6.53109E-02   4.75639E-01  -6.51675E-04   2.18901E-04   6.43500E-02
 -1.02016E-03  -2.95010E-01
HC21        BY          HC-3        300.0
  6.03969E-02   1.07719E+00  -4.06176E-02  -1.64803E-02   2.58807E-02
 -8.78938E-03  -8.72197E-01
HC32        BY          HC-3        300.0
  6.47026E-02   2.03998E+00  -9.78251E-02  -6.54136E-02   2.70146E-02
 -2.35901E-02  -1.62762E+00
HC43        BY          HC-3        300.0
  4.85596E-02  -1.63237E+00   1.59558E-01   4.72764E-02  -1.76932E-01
  3.68102E-02   1.48675E+00
HC54        BY          HC-3        300.0
  6.42262E-02   3.01016E-01   3.68099E-02  -1.81293E-03   2.81290E-02
  9.23514E-03  -1.34110E-01
HC65        BY          HC-3        300.0
  6.35112E-02   1.40087E+00  -5.71250E-02  -2.03039E-02   6.96926E-02
 -1.78970E-02  -1.15064E+00
HC76        BY          HC-3        300.0
  5.86701E-02  -6.31764E-01   8.79095E-02   4.58325E-02  -6.57527E-02
  2.00576E-02   6.31280E-01
HC87        BY          HC-3        300.0
  8.02417E-02   2.81480E+00  -2.05214E-01   2.60769E-02   2.01729E-01
 -7.56776E-02  -2.33427E+00
HC98        BY          HC-3        300.0
  6.18025E-02   1.90305E+00  -3.51234E-02  -7.26800E-02   5.71332E-02
 -3.28486E-02  -1.44251E+00
HC09        BY          HC-3        300.0
  6.60904E-02  -1.05653E+00   7.48716E-02   1.47456E-01  -1.39909E-01
 -8.68257E-03   1.07864E+00
HC10        BY          HC-0        400.0
  5.43550E-02   1.98845E-02   2.36386E-02   3.09269E-02  -2.41485E-02
  5.32499E-03   7.59366E-02
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HC21        BY         HC-0       400.0
   5.34164E-02   1.02781E-01   3.28273E-02   1.54700E-02  -1.01356E-02
   3.98248E-03  -1.37396E-03
HC32        BY         HC-0       400.0
   5.93131E-02   2.78068E+00  -1.26070E-01  -1.13495E-01   1.57950E-01
  -4.20559E-02  -2.33433E+00
HC43        BY         HC-0       400.0
   6.48433E-02   1.25805E+00  -7.55950E-02   1.45707E-02   1.09083E-01
  -3.39725E-02  -1.08723E+00
HC54        BY         HC-0       400.0
   5.47634E-02  -3.02808E-01   5.26607E-02   4.83423E-02  -1.04045E-01
   7.83965E-03   3.71801E-01
HC65        BY         HC-0       400.0
   5.64546E-02   1.75863E+00  -3.57133E-02  -7.91899E-02   8.39191E-02
  -2.56340E-02  -1.43700E+00
HC76        BY         HC-0       400.0
   5.14994E-02  -3.16648E-01   1.01904E-01   1.66846E-02  -1.10752E-01
   1.26710E-02   3.97852E-01
HC87        BY         HC-0       400.0
   6.20625E-02  -3.29181E-02   1.42866E-02   8.94451E-02  -5.93037E-02
  -2.05307E-02   1.19670E-01
HC98        BY         HC-0       400.0
   8.30708E-02  -3.09482E-02  -7.77838E-02   1.84396E-01  -6.12497E-02
  -3.99148E-02   1.53801E-01
HC09        BY         HC-0       400.0
   5.06195E-02  -1.03005E+00   1.76956E-01   1.73109E-02  -2.01417E-01
   2.54447E-02   1.03412E+00
HC10        BY         HC-1       400.0
   5.48654E-02   8.72384E-03   2.03293E-02   3.64266E-02  -2.89252E-02
   5.62153E-03   9.03833E-02
HC21        BY         HC-1       400.0
   5.51180E-02   1.33645E-02   2.44333E-02   3.55725E-02  -2.77429E-02
   5.09839E-03   8.62126E-02
HC32        BY         HC-1       400.0
   4.68490E-02  -8.25362E-01   1.17579E-01   2.38906E-02  -1.69441E-01
   2.83841E-02   8.07051E-01
HC43        BY         HC-1       400.0
   5.67451E-02   2.66886E+00  -9.11410E-02  -1.33458E-01   1.32187E-01
  -3.52754E-02  -2.22721E+00
HC54        BY         HC-1       400.0
   6.46308E-02   8.44169E-01  -4.70340E-02   3.60126E-02   6.14363E-02
  -2.51548E-02  -7.20696E-01
HC65        BY         HC-1       400.0
   5.78843E-02  -1.62178E-01   4.07230E-02   5.63021E-02  -1.06973E-01
   2.66719E-03   2.60990E-01
HC76        BY         HC-1       400.0
   5.69226E-02   2.30297E+00  -5.25581E-02  -1.07250E-01   1.57805E-01
  -4.16968E-02  -1.93686E+00
HC87        BY         HC-1       400.0
   6.86319E-02   1.00228E+00  -6.39406E-02   5.96576E-02   8.51572E-02
  -4.63765E-02  -8.54257E-01
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HC98        BY          HC-1       400.0
  6.82899E-02   -5.41201E-02    1.09289E-02    9.34992E-02   -6.85203E-02
 -2.00848E-02    1.65738E-01
HC09        BY          HC-1       400.0
  6.22341E-02   -1.36613E+00    1.02295E-01    1.54908E-01   -2.16815E-01
  3.36959E-04    1.33437E+00
HC10        BY          HC-2       400.0
  5.30508E-02    1.48114E-01    2.58280E-02    1.27799E-02   -3.49026E-03
  5.40569E-03   -3.83278E-02
HC21        BY          HC-2       400.0
  5.15849E-02   -1.39952E+00    1.01183E-01    1.05951E-01   -2.75230E-01
  2.89427E-02    1.35472E+00
HC32        BY          HC-2       400.0
  5.99338E-02    4.67127E-01   -2.14125E-02    3.72542E-02   -1.21154E-01
 -7.96931E-03   -2.43795E-01
HC43        BY          HC-2       400.0
  5.08636E-02   -1.29343E+00    1.19635E-01    7.97038E-02   -2.22692E-01
  2.66623E-02    1.23502E+00
HC54        BY          HC-2       400.0
  6.14671E-02    2.35304E+00   -9.13885E-02   -9.79780E-02    9.32765E-02
 -3.13164E-02   -1.94038E+00
HC65        BY          HC-2       400.0
  5.44608E-02   -2.46690E-01    7.15396E-02    2.78414E-02   -5.87680E-02
  7.33329E-03    2.43811E-01
HC76        BY          HC-2       400.0
  5.55762E-02    8.31561E-01    2.17848E-02   -2.38037E-02    1.53989E-02
 -1.71633E-02   -6.46497E-01
HC87        BY          HC-2       400.0
  6.88207E-02    2.50894E+00   -1.21037E-01   -4.50294E-02    2.20385E-01
 -6.95880E-02   -2.14592E+00
HC98        BY          HC-2       400.0
  7.65382E-02    1.37376E+00   -1.11724E-01    8.57287E-02    1.40464E-01
 -6.76887E-02   -1.19762E+00
HC09        BY          HC-2       400.0
  6.47061E-02   -7.06793E-01    6.15685E-02    1.26169E-01   -1.33819E-01
 -1.18931E-02    7.37797E-01
HC10        BY          HC-3       400.0
  5.46835E-02    2.43876E-01    1.07290E-02    1.87115E-02    1.41871E-02
 -1.07372E-03   -1.21170E-01
HC21        BY          HC-3       400.0
  3.94819E-02    4.56102E-01    1.03693E-01   -1.16138E-01   -1.10654E-01
  2.56675E-02   -2.73757E-01
HC32        BY          HC-3       400.0
  6.10318E-02   -1.02518E+00    3.40389E-02    1.47453E-01   -2.25982E-01
  4.63146E-03    1.03774E+00
HC43        BY          HC-3       400.0
  7.17678E-02    1.09026E+00   -1.11785E-01    7.80075E-02   -3.31199E-03
 -4.63041E-02   -8.30875E-01
HC54        BY          HC-3       400.0
  3.42896E-02   -1.54227E+00    2.18714E-01    1.27938E-02   -2.76848E-01
  4.71397E-02    1.46864E+00
```

HC65	BY	HC-3	400.0	
5.76125E-02	2.90388E-01	2.33915E-02	3.18454E-02	2.60828E-03
-8.84707E-03	-1.56180E-01			
HC76	BY	HC-3	400.0	
6.05672E-02	1.61278E-01	1.41709E-02	6.25860E-02	-4.54218E-02
-1.11174E-02	-8.73830E-02			
HC87	BY	HC-3	400.0	
4.19811E-02	4.80138E-01	1.21486E-01	-9.16294E-02	-2.93920E-02
6.96809E-03	-3.40422E-01			
HC98	BY	HC-3	400.0	
7.74424E-02	2.82716E+00	-1.69941E-01	-3.61212E-02	2.67061E-01
-8.05388E-02	-2.43258E+00			
HC09	BY	HC-3	400.0	
7.30037E-02	8.29926E-01	-7.48573E-02	1.11411E-01	5.95236E-02
-5.63138E-02	-6.58711E-01			
HC10	BY	HC-0	500.0	
4.77462E-02	1.55645E-02	2.54955E-02	3.15638E-02	-3.04526E-02
1.52178E-04	6.15941E-02			
HC21	BY	HC-0	500.0	
4.70022E-02	5.59751E-01	1.32655E-02	-2.14774E-02	1.84716E-02
-3.43051E-03	-4.63124E-01			
HC32	BY	HC-0	500.0	
6.05799E-02	2.36501E+00	-1.42052E-01	-4.67586E-02	1.40903E-01
-4.80593E-02	-1.99016E+00			
HC43	BY	HC-0	500.0	
4.59753E-02	7.33918E-01	2.50681E-02	-3.44873E-02	-2.62245E-03
-1.03217E-02	-5.83889E-01			
HC54	BY	HC-0	500.0	
5.44115E-02	4.29724E-01	-4.39796E-03	3.40090E-02	4.00635E-04
-1.40825E-02	-3.60440E-01			
HC65	BY	HC-0	500.0	
5.41200E-02	-4.99427E-01	5.38519E-02	6.75420E-02	-1.10353E-01
6.96327E-03	4.91497E-01			
HC76	BY	HC-0	500.0	
4.79630E-02	9.44629E-01	2.38827E-02	-3.80217E-02	3.70577E-02
-1.96779E-02	-7.80997E-01			
HC87	BY	HC-0	500.0	
5.18731E-02	3.01214E-01	4.15168E-02	1.84191E-02	-1.49783E-02
-1.80933E-02	-2.06600E-01			
HC98	BY	HC-0	500.0	
4.59244E-02	-5.15063E-01	1.26473E-01	2.41653E-02	-1.18731E-01
2.61360E-03	5.38302E-01			
HC09	BY	HC-0	500.0	
4.55170E-02	1.69269E-01	1.12046E-01	-3.45586E-02	-6.39027E-02
-4.20859E-03	-5.86524E-02			
HC10	BY	HC-1	500.0	
4.82755E-02	9.88887E-03	2.16061E-02	3.73994E-02	-3.34400E-02
-1.34450E-04	7.02531E-02			
HC21	BY	HC-1	500.0	
4.83665E-02	1.81930E-02	2.70933E-02	3.43617E-02	-3.27866E-02
-3.61147E-04	6.23419E-02			

```
HC32        BY        HC-1      500.0
 3.85774E-02   4.31806E-01   6.32056E-02  -5.21512E-02  -6.17334E-02
 5.66679E-03  -3.01538E-01
HC43        BY        HC-1      500.0
 6.32020E-02   3.46421E+00  -2.15224E-01  -6.93958E-02   2.40099E-01
-7.76987E-02  -2.94907E+00
HC54        BY        HC-1      500.0
 5.04039E-02   6.68931E-01  -2.73957E-03   1.22510E-02   2.35022E-02
-1.96473E-02  -5.53189E-01
HC65        BY        HC-1      500.0
 5.02673E-02  -7.41785E-02   3.18977E-02   6.21762E-02  -4.52902E-02
-7.85286E-03   8.61451E-02
HC76        BY        HC-1      500.0
 4.38696E-02  -1.69187E-01   9.77770E-02  -1.10386E-03  -8.72596E-02
 8.25914E-03   2.12707E-01
HC87        BY        HC-1      500.0
 5.08926E-02   1.19024E+00  -7.96675E-03  -2.33576E-02   5.83197E-02
-3.23471E-02  -9.80202E-01
HC98        BY        HC-1      500.0
 4.80914E-02   4.30463E-01   6.57747E-02  -1.71606E-02  -1.04916E-02
-1.53400E-02  -3.01374E-01
HC09        BY        HC-1      500.0
 5.61397E-02  -2.12714E-01   6.65382E-02   5.26857E-02  -8.74997E-02
-1.02222E-02   2.77953E-01
HC10        BY        HC-2      500.0
 4.72411E-02   6.53413E-02   2.56518E-02   2.46918E-02  -2.21396E-02
 1.07333E-03   1.92198E-02
HC21        BY        HC-2      500.0
 4.77437E-02   3.25049E-01  -2.28120E-03   3.58716E-02  -4.24031E-02
-8.23362E-03  -2.31881E-01
HC32        BY        HC-2      500.0
 4.79784E-02  -4.90076E-01   4.00136E-02   8.41002E-02  -1.32071E-01
 1.23790E-03   5.03971E-01
HC43        BY        HC-2      500.0
 3.75518E-02  -6.28680E-01   1.26882E-01  -1.90114E-03  -1.57755E-01
 2.43593E-02   6.24196E-01
HC54        BY        HC-2      500.0
 4.47223E-02   1.92863E+00  -1.88441E-02  -1.19255E-01   7.81696E-02
-2.32383E-02  -1.60405E+00
HC65        BY        HC-2      500.0
 5.04186E-02   7.15599E-01   7.35285E-04   1.26134E-02   2.60517E-02
-2.12419E-02  -6.02802E-01
HC76        BY        HC-2      500.0
 4.95898E-02   4.86520E-02   4.54207E-02   4.14611E-02  -4.32073E-02
-8.52061E-03  -8.34006E-03
HC87        BY        HC-2      500.0
 4.24045E-02   6.45369E-01   6.21326E-02  -3.56373E-02   1.59008E-02
-1.44942E-02  -5.38141E-01
HC98        BY        HC-2      500.0
 5.85668E-02   1.64521E+00  -4.57051E-02  -3.08567E-02   1.02252E-01
-4.32911E-02  -1.38180E+00
```

```
HC09        BY        HC-2      500.0
  4.34181E-02  -6.89569E-01   1.48559E-01   2.67038E-02  -1.10247E-01
  6.48016E-03   6.49585E-01
HC10        BY        HC-3      500.0
  4.79058E-02   1.57218E-01   1.62716E-02   2.52479E-02  -6.82747E-03
 -2.91680E-03  -6.16589E-02
HC21        BY        HC-3      500.0
  3.71911E-02  -4.33406E-01   1.02654E-01  -1.71799E-03  -1.23417E-01
  1.88092E-02   4.45318E-01
HC32        BY        HC-3      500.0
  4.86234E-02  -1.00084E+00   6.67103E-02   1.15542E-01  -1.60207E-01
  6.51760E-03   9.26002E-01
HC43        BY        HC-3      500.0
  5.03310E-02   3.77307E-01  -5.33411E-03   3.72167E-02  -9.69520E-02
 -9.86138E-03  -2.13109E-01
HC54        BY        HC-3      500.0
  3.87809E-02   4.97973E-01   8.16179E-02  -7.80218E-02  -9.86827E-02
  1.12513E-02  -3.22344E-01
HC65        BY        HC-3      500.0
  4.71961E-02   1.60623E+00  -9.07931E-03  -8.41972E-02   6.00481E-02
 -2.38439E-02  -1.33984E+00
HC76        BY        HC-3      500.0
  5.49345E-02   9.12271E-01  -1.46355E-02   2.94738E-03   3.78188E-02
 -2.46991E-02  -7.60242E-01
HC87        BY        HC-3      500.0
  4.34950E-02   7.95144E-01   6.40181E-02  -6.87873E-02   4.61000E-03
 -7.18384E-03  -6.19732E-01
HC98        BY        HC-3      500.0
  4.67469E-02   1.17267E+00   3.61529E-02  -6.25254E-02   5.69120E-02
 -2.50409E-02  -9.81449E-01
HC09        BY        HC-3      500.0
  5.02303E-02   5.46384E-01   5.27197E-02  -4.17842E-03  -1.39539E-02
 -2.16554E-02  -3.88600E-01
HC10        BY        H2        200.0
 L-S FIT COEFFICIENTS  C(0)... C(ND)
  4.71013E-02   1.24132E-01   1.12012E-02  -3.26742E-02   2.49585E-02
 -1.16688E-04  -4.32674E-02
HC10        BY        H2        300.0
 L-S FIT COEFFICIENTS  C(0)... C(ND)
  3.02429E-02   1.88877E-01  -4.06585E-03  -1.66012E-02   2.40520E-02
 -3.04313E-03  -1.25203E-01
HC10        BY        H2        400.0
 L-S FIT COEFFICIENTS  C(0)... C(ND)
  2.29643E-02   1.38503E-01  -3.30824E-03  -9.67516E-03   1.74500E-02
 -2.56123E-03  -1.00183E-01
HC10        BY        H2        500.0
 L-S FIT COEFFICIENTS  C(0)... C(ND)
  1.99680E-02   7.67147E-02   5.07801E-04  -7.65486E-03   1.00916E-02
 -1.02944E-03  -5.70837E-02
```

```
HC10        BY        AR        200.0
 L-S FIT COEFFICIENTS  C(0)... C(ND)
  1.14354E-01   5.09231E-01  -3.37538E-01   1.98076E-01  -4.12480E-03
 -2.79543E-02  -2.79080E-01
HC10        BY        AR        300.0
 L-S FIT COEFFICIENTS  C(0)... C(ND)
  1.31036E-01  -2.10514E-02  -3.33416E-01   2.28662E-01  -2.29148E-02
 -1.74768E-02   1.13322E-01
HC10        BY        AR        400.0
 L-S FIT COEFFICIENTS  C(0)... C(ND)
  2.25690E-01  -4.41998E-01  -5.14261E-01   3.61613E-01  -4.24690E-02
 -1.69524E-02   4.45504E-01
HC10        BY        AR        500.0
 L-S FIT COEFFICIENTS  C(0)... C(ND)
  2.62995E-01  -6.43115E-01  -5.82478E-01   4.13800E-01  -5.44508E-02
 -1.56157E-02   6.05413E-01
```

APPENDIX 3

LINEWIDTH EVALUATION SUBROUTINE AND SAMPLE TEST PROGRAM

```
      FUNCTION GAMMA2(PTOT,TKEN,CLS,NCLS,CNLS,NCNLS,CSA,NCSA,LV,M)
      COMMON COFT(5,7,10,4),CNOFT(5,7,2),CAOFT(5,7,1),NPL,NVL,NPNL,NPA
      DIMENSION CNLS(5),TS(5),CLS(5),CSA(5),P(15)
C  CALCULATE PARTIAL PRESSURES FOR EACH PERTURBING SPECIES
      DO 1 I=1,NCLS
      IF(I.LT.NPL) P(I)=PTOT*CLS(I)
1     IF(I.GE.NPL) P(NPL)=P(NPL)+PTOT*CLS(I)
      DO 2 I=1,NCNLS
      IF(I.LT.NPNL) P(NPL+I)=PTOT*CNLS(I)
2     IF(I.GE.NPNL) P(NPL+NPNL)=P(NPL+NPNL)+PTOT*CNLS(I)
      DO 3 I=1,NCSA
      IF(I.LT.NPA) P(NPL+NPNL+I)=PTOT*CSA(I)
3     IF(I.GE.NPA) P(NPL+NPNL+NPA)=P(NPL+NPNL+NPA)+PTOT*CSA(I)
C  FIND TEMPERATURE RANGE
      DO 4 J=2,NT
      IF(TS(J).LT.TKEN)GO TO 4
      T1=TS(J-1)
      T2=TS(J)
      I1=J-1
      I2=J
      GO TO 5
4     CONTINUE
C
5     CONTINUE
103   FORMAT(1X,1PE14.5)
      XM=FLOAT(M)
      F24=EXP(-XM/4.)
      F34=XM*EXP(-XM/4.)
      F44=(XM**2)*EXP(-XM/2.)
```

```
      F5M=XM*EXP(-XM**2/8.)
      F6M=(XM**2)*EXP(-XM**2/16.)
      F7M=EXP(-XM**2/8.)
      IF(I2.EQ.IKEN)GO TO 9
C   CALCULATE GT1
      GT1=0.
      DO 7 I=1,NPI
      GT1=GT1+P(I)*(COFT(I1,1,IV,I)+
     1 COFT(I1,2,IV,I)*F2M+COFT(I1,3,IV,I)*F3M+COFT(I1,4,IV,I)*F4M+
     1 COFT(I1,5,IV,I)*F5M+COFT(I1,6,IV,I)*F6M+COFT(I1,7,IV,I)*F7M)
7     CONTINUE
      DO 17 I=1,NPNI
      GT1=GT1+P(I)*(CNOFT(I1,1,I)+
     1 CNOFT(I1,2,I)*F2M+CNOFT(I1,3,I)*F3M+CNOFT(I1,4,I)*F4M+
     1 CNOFT(I1,5,I)*F5M+CNOFT(I1,6,I)*F6M+CNOFT(I1,7,I)*F7M)
17    CONTINUE
      DO 27 I=1,NPA
      GT1=GT1+P(I)*(CAOFT(I1,1,I)+
     1 CAOFT(I1,2,I)*F2M+CAOFT(I1,3,I)*F3M+CAOFT(I1,4,I)*F4M+
     1 CAOFT(I1,5,I)*F5M+CAOFT(I1,6,I)*F6M+CAOFT(I1,7,I)*F7M)
27    CONTINUE
      IF(I1.NE.IKEN)GO TO 9
C   IF I1=IKEN THEN GAMMA=GT1
      GAMMA2=GT1
      RETURN
C   CALCULATE GT2
9     GT2=0.
      DO 19 I=1,NC
      GT2=GT2+P(I)*(COFT(I2,1,IV,I)+
     1 COFT(I2,2,IV,I)*F2M+COFT(I2,3,IV,I)*F3M+COFT(I2,4,IV,I)*F4M+
     1 COFT(I2,5,IV,I)*F5M+COFT(I2,6,IV,I)*F6M+COFT(I2,7,IV,I)*F7M)
19    CONTINUE
      IF(I2.NE.IKEN)GO TO 30
C   IF I2=IKEN THEN GAMMA=GT2
      GAMMA2=GT2
      RETURN
```

```
C   INTERPOLATE GT1 AND GT2 TO GET GAMMA
30      GAMMA2=(ALOG(GT2)-ALOG(GT1))/(ALOG(T2)-ALOG(T1))
        GAMMA2=GT1*EXP(GAMMA2*(ALOG(TKEN)-ALOG(T1)))
        RETURN
        END
        COMMON COFT(5,7,10,4),CNOFT(5,7,2),CAOFT(5,7,1),NPL,NVL,NPNL,NPA
        DIMENSION CNLS(5),TS(5),CLS(5),CSA(5)
        READ(3,100)PTOT,NCLS,NCNLS,NCSA
        READ(3,101) (CLS(I),I=1,NCLS)
        READ(3,101) (CNLS(I),I=1,NCNLS)
        READ(3,101) (CSA(I),I=1,NCSA)
        READ(5,102) NT,(TS(I),I=1,NT)
        READ(5,104)NPL,NVL
        DO 16 N=1,NT
        DO 16 I=1,NPL
        DO 16 LV=1,NVL
16      READ(5,103) (COFT(N,J,LV,I),J=1,7)
        READ(5,104)NPNL
        DO 116 N=1,NT
        DO 116 I=1,NPNL
116     READ(5,103) (CNOFT(N,J,I),J=1,7)
        READ(5,104)NPA
        DO 216 N=1,NT
        DO 216 I=1,NPA
216     READ(5,103) (CAOFT(N,J,I),J=1,7)
        DO 1 LV=1,10
        DO 1 M=1,5
        G=GAMMA2(PTOT,TKEN,CLS,NCLS,CNLS,NCNLS,CSA,NCSA,LV,M)
1       WRITE(6,105)M,G
100     FORMAT(1X,F5.4,3I2)
101     FORMAT(1X,5F4.2)
102     FORMAT(1X,I2,6F4.0)
103     FORMAT(1X,1P5E14.5)
104     FORMAT(1X,I2)
105     FORMAT(1X,'GAMMA(',I2,')=',F10.4)
```

APPENDIX 4

CHEMISTRY CODE LISTINGS

```
      SUBROUTINE CHEMS
C  *** HOFER'S CHEMISTRY CODE, MODIFIED BY TUER (3/23/77).
      REAL MWT
      INTEGER RTYP,RCTP,RSPE,REACT,RLP,RRP,SPECIE,SPLP,SPRP,AID
      DIMENSION REACT(225,6),RLP(225,6),IRCT(225,6),RRP(225,6),
     +HF(50)
      COMMON/THERMO/TTB(24),GTB(50,24),CPTB(50,24),HTB(50,24)
      DIMENSION STB( 50,24)
      DATA IBLANK/'   '/,R1/82.057/
      EQUIVALENCE (STB,GTB)
      DIMENSION IVT(5,30),NVT(5)
      COMMON/SPECYS/ALPHA(50),G(50)
      COMMON/IDENT/AID(50),SPLP(50),ISPEC(50),SPRP(50)
      EQUIVALENCE (SPECIE,AID)
      COMMON/RATE/RCON(225,7),WDOT(50),RA(225),IRT(225),
     +IR(50,225),IL(50,225),KR(225,3),KL(225,3),
     +RSPE(225,6),IFLAG(10)
      COMMON/KON1/CNU(50),NST,NALL,NSPALL,NRT,NT,WE(2),WEXE(2)
     +,MWT(50)
      EQUIVALENCE (IRT,RTYP)
      DIMENSION RCTP(225),RTYP(225),SPECIE(50)
C     MAIN PGRAM FOR HEL
C     IFLAG(1)=1 PRINT OUT THERMO DATA
C     IFLAG(2)=1 PRINT OUT REACTIONS
C     IFLAG(3)=1 PRINT OUT INITIAL CONCENTRATIONS
C     IFLAG(4)=1 PRINT OUT RA(J) AND RV(J)
C     IFLAG(5)=1 PRINT OUT RP(J) AND RM(J)
      READ(5,100)NST,NRT,NT,NALL,(IFLAG(I),I=1,10)
 100  FORMAT(4I5,5X,10I1)
      WRITE(6,1009) NST,NRT,NT,NALL,(IFLAG(I),I=1,10)
 1009 FORMAT(' NST=',I5,2X,'NRT=',I5,2X,'NT=',I5,2X,'NALL=',I5,2X,
     1 'NUM=',I5,2X,'IFLAG=',10I1)
C     ***** INPUT SPECIES THERMO DATA *****
C     ONLY 99 SPECIES CAN BE CONSIDERED
      NSPALL=NST+NALL
      DO 9 NS=1,NSPALL
      DO 9 NR=1,NRT
      IR(NS,NR)=0
      IL(NS,NR)=0
    9 CONTINUE
C     THE CATALYTIC SPECIES WHICH ARE DESIGNATED AS "ALL" IN THE
C     PARENTHESIS(E.G. HCL(ALL)) MUST BE THE LAST SPECIES IN THE
C     THERMO DATA
      DO 10 NS=1,NSPALL
      READ(5,300) SPECIE(NS),SPLP(NS),ISPEC(NS),SPRP(NS),MWT(NS),HF(NS)
  300 FORMAT(A3,A1,I3,A1,2F10.3)
      DO 11 IT=1,NT,2
      READ(5,301) TTB(IT),CPTB(NS,IT),STB(NS,IT),HTB(NS,IT),
     1TTB(IT+1),CPTB(NS,IT+1),STB(NS,IT+1),HTB(NS,IT+1)
  301 FORMAT(8F10.3)
   11 CONTINUE
```

```
   10 CONTINUE
      IF(IFLAG(1).EQ.0) GO TO 13
      WRITE(6,302)
  302 FORMAT(1H1,' THERMO DATA FOR SPECIES CONSIDERED IN THIS RUN')
      DO 12 NS=1,NSPALL
      WRITE(6,303) SPECIE(NS),SPLP(NS),ISPEC(NS),SPRP(NS),MWT(NS),HF(NS)
  303 FORMAT(1X,A3,A1,I3,A1,2F10.3)
      DO 12 IT=1,NT,2
      WRITE(6,304) TTB(IT),CPTB(NS,IT),STB(NS,IT),HTB(NS,IT),
     1TTB(IT+1),CPTB(NS,IT+1),STB(NS,IT+1),HTB(NS,IT+1)
  304 FORMAT(1X,2(F10.0,3F10.3))
   12 CONTINUE
   13 CONTINUE
C     THE KL AND KR MATRIX HAS THE COEFFICIENTS FOR THE VARIOUS
C     REACTIONS-NOTE KL IS FOR SPECIES ON THE LEFT SIDE OF THE = SIGN
C     AND THE KR IS FOR THE SPECIES ON THE RIGHT SIDE OF THE = SIGN
C     EXAMPLE OF KL AND KR
C     KL(J,1)HCL + KL(J,2)H2 +      = KR(J,1)HCL +KR(J,2)H2 +
C     WHERE J DESIGNATES THE REACTION OF INTEREST
C     THE MATRIX IL AND IR IS DIMENSIONED(NUMBER OF SPECIES, NUMBER OF
C     REACTIONS) AND IS USED IN THE CHEMISTRY SUBROUTINE TO COMPUTE WDOT
C     THE ELEMENT OF THE IL AND IR MATRIX WHICH ARE NON-ZERO
C     ARE THE SPECIES WHICH ARE PRESENT IN THAT PARTICULAR REACTION.
C     THE NUMERICAL VALUE IS INDICATIVE OF THE NUMBER OF MOLES PRESENT
C     IN THAT PARTICULAR REACTION.
C     RCTP IS THE PARAMETER TO TREAT REVERSIBLE OF NON-REVERSIBLE
C     REACTIONS.
C     RTYP IS USED TO DETERMINE THE FORM OF THE RATE EQUATION
C     RSPE IS A MATRIX WHICH CONTAINS THE NUMBER OF THE SPECIE RELATIVE
C     TO THE ORDER IN THE THERMO DATA FOR EACH REACTION WITH 3 REACTANTS
C     AND 3 PRODUCTS
      DO 23 NS=1,NSPALL
      DO 23 IT=1,NT
      HTB(NS,IT)=(HTB(NS,IT)+HF(NS))*1000.
      GTB(NS,IT)=HTB(NS,IT)-TTB(IT)*STB(NS,IT)
   23 CONTINUE
C     ***** INPUT REACTION RATES AND REACTIONS *****
      DO 2600 J=1,NRT
      READ(5,1400) (KL(J,K),REACT(J,K),RLP(J,K),IRCT(J,K),
     1RRP(J,K),K=1,3),(KR(J,K-3),REACT(J,K),RLP(J,K),IRCT(J,K),
     2RRP(J,K),K=4,6)
 1400 FORMAT(6(I1,A3,A1,I3,A1,1X),20X)
      READ(5,1401) RCTP(J ),RTYP(J ),(RCON(J ,K),K=1,7)
 1401 FORMAT(I1,I2,1X,2F3.1,20X,E10.3,F10.3,E10.3,F10.3,F10.3)
C     THE VECTOR RSPE HAS THE NUMBER OF THE SPECIE FROM THE ORDER OF
C     THE THERMO DATA
C     THE REACTION RATES ARE IN CM**3/(PARTICLE*SECONDS)
      DO 2600 K=1,6
      IF(REACT(J ,K).NE.IBLANK) GO TO 2400
      RSPE(J ,K)=-1
```

```
      IF(K.LE.3) KL(J ,K)=0
      IF(K.GE.4) KR(J ,K-3)=0
      GO TO 2600
 2400 DO 2500 I=1,NSPALL
      IF(SPECIE(I ).NE.REACT(J ,K).OR.ISPEC(I).NE.IRCT(J,K)) GO TO 2500
      RSPE(J ,K)=I
      IF(K.LE.3) IL(I ,J )=KL(J ,K)
      IF(K.GE.4) IR(I ,J )=KR(J ,K-3)
C     GENERATE IL AND IR MATRIX
      GO TO 2600
 2500 CONTINUE
      WRITE(6,1402) REACT(J,K)
 1402 FORMAT(1X,' SPECIE ',A8,' NOT FOUND IN DATA BASE')
 2600 CONTINUE
      IF(IFLAG(2).EQ.0) GO TO 2800
      WRITE(6,1403)
 1403 FORMAT(1H1,' REACTIONS AND RATE CONSTANTS USED IN THIS CASE ')
      DO 170 J=1,NRT
      WRITE(6,1404)  J ,(KL(J ,K),REACT(J ,K),RLP(J,K),IRCT(J,K),
     +RRP(J,K),K=1,3),
     +(KR(J ,K-3),REACT(J ,K),RLP(J,K),IRCT(J,K),RRP(J,K),K=4,6),
     +RCTP(J ),RTYP(J )
  170 CONTINUE
 1404 FORMAT(1X,I3,1X,I1,A3,A1,I3,A1,2('+',I1,A3,A1,I3,A1),'=',
     +I1,A3,A1,I3,A1,2('+',I1,A3,A1,I3,A1),1X,I2,1X,I2)
      WRITE(6,1500)
 1500 FORMAT(1H1)
      DO 2700 J=1,NRT
      IF(RTYP(J).EQ.1)
     +WRITE(6,1501) J,RCON(J,1),RCON(J,3),RCON(J,4)
 1501 FORMAT(1X,I3,1X,F3.0,'*',E10.3,'EXP(',F10.3,'/T)')
      IF(RTYP(J).EQ.2)
     +WRITE(6,1502) J,RCON(J,2),RCON(J,3),RCON(J,4)
 1502 FORMAT(1X,I3,1X,F3.0,'*',E10.3,'EXP(',F10.3,'/T)')
      IF(RTYP(J).EQ.3) GO TO 2700
      IF(RTYP(J).EQ.4)
     +WRITE(6,1504) J,RCON(J,2),RCON(J,3),RCON(J,4)
 1504 FORMAT(1X,I3,1X,F3.0,'*',E10.3,'*EXP(',F10.3,'*DE23*T**1/3)')
      IF(RTYP(J).EQ.5)
     +WRITE(6,1505) J,RCON(J,1),RCON(J,3),RCON(J,5),RCON(J,6)
 1505 FORMAT(1X,I3,1X,F3.0,'*(',E10.3,'+',E10.3,'*EXP(',F10.3,'*DE23*T**
     +1/3)')
      IF(RTYP(J).EQ.6) GO TO 2700
      IF(RTYP(J).EQ.7)
     +WRITE(6,1507) J,RCON(J,1),RCON(J,3),RCON(J,4),RCON(J,5),RCON(J,6)
 1507 FORMAT(1X,I3,1X,F3.0,'*(',E10.3,'*EXP(',F10.3,'*DE23*T13)+',E10.3,
     +'*EXP(',F10.3,'*T13))')
      IF(RTYP(J).EQ.8) GO TO 2700
      IF(RTYP(J).EQ.9)
     +WRITE(6,1509) J,RCON(J,1),RCON(J,2),RCON(J,3),RCON(J,5),RCON(J,6)
```

```
 1509 FORMAT(1X,I3,1X,F3.0,'*',F3.0,'*(',E10.3,'+',E10.3,'*EXP(',F10.3,'
     +*DE23*T**-1/3))')
      IF(RTYP(J).EQ.10)
     +WRITE(6,1510)J,RCON(J,1),RCON(J,2),RCON(J,3),RCON(J,4),RCON(J,5),
     +RCON(J,6),RCON(J,7)
 1510 FORMAT(1X,I3,1X,F3.0,'*',F3.0,'*(',E10.3,'*T**-.5*EXP(',F10.3,'*DE
     +)+',E10.3,'*T**.5*EXP(-(',F10.3,'*DE23+',F10.3,')*T**-1/3)')
      IF(RTYP(J).EQ.11)
     +WRITE(6,1511) J,RCON(J,1),RCON(J,2),RCON(J,3),RCON(J,4),RCON(J,5),
     +RCON(J,6),RCON(J,7)
 1511 FORMAT(1X,I3,1X,F3.0,'*',F3.0,'*(',E10.3,'*T**-.5*EXP(',F10.3,'*DE
     ++',E10.3,'*T**.5*EXP(',F10.3,'*DE23+',F10.3,')*T**-1/3)')
 2700 CONTINUE
 2800 CONTINUE
      READ(5,599)  (WE(I),WEXE(I),I=1,2)
  599 FORMAT(4F10.8)
      READ(5,600)  (CNU(NS),NS=1,NST)
  600 FORMAT(7E10.3)
      IF(IFLAG(3).EQ.0)GO TO 18
      WRITE(6,601)
  601 FORMAT(1H1,' INITIAL CONCENTRATIONS OF SPECIES IN MOLE ',
     1 'FRACTIONS AT NOZZLE')
      WRITE(6,602)  (SPECIE(NS),SPLP(NS),ISPEC(NS),SPRP(NS),CNU(NS),NS=1,NST)
  602 FORMAT(3(2X,A3,A1,I3,A1,'=',1PE11.4))
   18 CONTINUE
C     CONVERT FROM MOLE FRACTION TO MOLES/CC
      CNTI=0.0
      WTVR=0.0
C     WTVR IS IN UNITS GRAMS GAS /MOLES GAS
      DO 19 NS=1,NST
      WTVR=WTVR+CNU(NS)*MWT(NS)
C     MUST HAVE NON-ZERO CONCENTRATION FOR RATE OF PRODUCTION OF SPECIES
C     EQUATIONS TO WORK PROPERLY
      CNTI=CNTI+CNU(NS)
   19 CONTINUE
      WRITE(6,603) CNTI
  603 FORMAT(1H0,' THE TOTAL MOLE FRACTION =',F10.8)
      CALL CHEMVI(IVI,NVT)
      RETURN
      ENTRY CHEM(T,P,DT)
      WRITE(6,611) T,P,DT
  611 FORMAT(1H1,' TEMPERATURE =',1PE11.4,2X,'PRESSURE(ATM) =',
     +1PE11.4,2X,'DELTA TIME =',1PE11.4)
C     RHO IS IN UNITS GRAMS GAS/CM**3
      RHO=P*WTVR/(T*R1)
      WRITE(6,607) RHO,WTVR,SUMDT
  607 FORMAT(2X,'RHO =',1PE11.4,5X,'MOLECULAR WEIGHT OF GAS =',
     +1PE11.4,5X,'SUM DELTA TIME=',1PE11.4)
      DO 20 NS1=1,NST
      IF(CNU(NS1).LE.0.0) CNU(NS1)=1.0E-50
      ALPHA(NS1)=CNU(NS1)/WTVR
```

AD-A044 625 SCIENCE APPLICATIONS INC ANN ARBOR MICH F/G 20/5
LINEWIDTH AND CHEMISTRY MODELING OF THE HCL-H2 NON-REACTING MIX--ETC(U)
AUG 77 F G SMITH, R E MEREDITH DAAK40-76-C-0754
UNCLASSIFIED SAI-77-003-AA NL

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C     CN NOW IS CONVERT FRCM MOLE FRACTION TO MOLES/GM GAS
   20 ALPHA(NS1)=ALPHA(NS1)*RHC
C     CN AND ALPHA ARE NOW IN UNITS OF MOLES I/CM**3
      CALL CHMSUM(IVT,NVT,ALPHA(1))
      WRITE(6,608)
  608 FORMAT(1H0,' INITIAL CCNCENTRATIONS OF SPECIES IN MOLES/CM**3')
      WRITE(6,602)  (SPECIE(NS),SPLP(NS),ISPEC(NS),SPRP(NS),
     +ALPHA(NS),NS=1,NSPALL)
      CALL CHMSTY(T,ALPHA(1))
      WRITE(6,610)
  610 FORMAT(1H1)
      WRITE(6,609)
  609 FORMAT(2X,'SPECIE',8X,'CNU',21X,'WDOT'/
     115X,'(MOLE',19X,'(MOLES/'/
     213X,'FRACTIONS)',14X,'MOLES-SEC)')
      DO 21 NS2=1,NST
C     WDOT IS IN UNITS MOLES I/(CM**3-SECOND)
C     WDOT IS NOW CONVERTED TO UNITS MOLES I/(MOLES-SEC)
      WDOT(NS2)=WDOT(NS2)*WTVR/RHO
      CNU(NS2)=CNU(NS2)+WDCT(NS2)*DT
      IF(CNU(NS2).LT.0.0) CNU(NS2)=1.0E-50
      WRITE(6,605) SPECIE(NS2),SPLP(NS2),ISPEC(NS2),SPRP(NS2),
     +CNU(NS2),WDCT(NS2)
  605 FORMAT(1X,A3,A1,I3,A1,'=',1PE15.8,10X,1PE15.8)
   21 CONTINUE
      WRITE(6,612)
      RETURN
  612 FORMAT(1H0,' CONCENTRATICNS OF SPECIES IN MOLE FRACTIONS AT DELTA TIME')
      WRITE(6,606) (SPECIE(NS),SPLP(NS),ISPEC(NS),SPRP(NS),
     +CNU(NS),NS=1,NSPALL)
  606 FORMAT(3(1X,A3,A1,I3,A1,'=',1PE11.4))
      END
      SUBROUTINE CHEMVI(IVT,NVT)
      INTEGER SPECIE,SPLP,SPRP,AID
      COMMON/IDENT/AID(50),SPLP(50),ISPEC(50),SPRP(50)
      COMMON/KON1/CNU(50),NST,NALL,NSPALL,NRT,NT,WE(2),WEXE(2)
     +,MWT(50)
C     THIS SUBROUTINE CALCULATES THE ARRAYS USED TO COMPUTE
C     THE SUMS OF CONCENTRATIONS IN THE VT DEACTIVATION PROCESS
C     M IS THE SPECIE WHICH IS TO BE ADDED TO THE "ALL" COMPOUNDS
C     L IS THE "ALL" COMPOUNDS POSITICN IN ARRAY IVT
C     NVT IS THE NUMBER OF SPECIES THAT WILL CONTRIBUTE TO THE "ALL"
C     COMPOUND
      DIMENSION IVT(5,30),NVT(5),IAI(8)
      DIMENSION SPECIE(1)
      EQUIVALENCE (SPECIE,AID)
      DATA ILPARN/1H(/,IALL/999/,L/0/
C     NOTE ALL SPECIES WITH ALL IN THE FORMULA MUST BE AT THE END
C     OF THE THERMODYNAMIC DATA
      NSP1=NST+1
      DO 6 I=NSP1,NSPALL
```

```
C       DECODE(8,100,SPECIE(I))  (IAI(K),K=1,8)
C  101  FORMAT(1X,A8,8(1X,A1))
C  100  FORMAT(8A1)
C       DO 1 I1=1,8
C       J=I1
        IF(SPLP(I).EQ.ILPARN) GC TO 2
     1  CONTINUE
        WRITE(10,1000) SPECIE(I)
  1000  FORMAT(1X,A3,A1,I3,A1,'THE SPECIE DOES NOT HAVE PROPER LABEL')
        GO TO 6
     2  IF(ISPEC(I).EQ.IALL)GC TC 3
        WRITE(10,1000) SPECIE(I),SPLP(I),ISPEC(I),SPRP(I)
C       THE LAST SPECIE WITH ALL IN ITS FORMULA HAS BEEN FOUND
        GO TO 6
     3  CONTINUE
        L=L+1
C       IF(J.EQ.3) ENCODE(2,205,ICHAR) (IAI(K),K=1,2)
C  205  FORMAT(2A1)
C  200  FORMAT(A2)
C       IF(J.EQ.4) ENCODE(3,305,ICHAR) (IAI(K),K=1,3)
C  305  FORMAT(3A1)
C  300  FORMAT(A3)
        N=0
        DO 5 M=1,NST
C       IF(J.EQ.3) DECODE(2,200,SPECIE(M)) ICHAR1
C       IF(J.EQ.4) DECODE(3,300,SPECIE(M)) ICHAR1
        IF(SPECIE(M).EQ.SPECIE(I)) GO TO 4
        GO TO 5
     4  N=N+1
        IVT(L,N)=M
     5  CONTINUE
        NVT(L)=N
     6  CONTINUE
     7  RETURN
        END
        SUBROUTINE CHMSUM(IVT,NVT,CN)
        DIMENSION CN(1)
        COMMON/KON1/CNU(50),NST,NALL,NSPALL,NRT,NT,WE(2),WEXE(2)
       +,MWT(50)
        DIMENSION IVT(5,30),NVT(5)
C       THIS SUBROUTINE COMPUTES CONCENTRATIONS FOR THE COMPOSITE
C       COMPOUNDS
C       III=NST*(LL-1)
        DO 2 I=1,NALL
        L=NST+I
        CN(L)=0.0
        N=NVT(I)
        DO 1 K=1,N
     1  CN(L)=CN(L)+CN(IVT(I,K))
     2  CONTINUE
        RETURN
        END
```

```
      SUBROUTINE CHMSTY(T,CN)
C          *****  SUBPROGRAM 1 - CHEMISTRY  *****
C    *** UNITS=KILCCALORIES,MOLES,CUBIC CENTIMETERS,SECONDS,DEGREES KELVIN ***
C     *** INPUT = CN-MIXED SPECIES CONCENTRATION (MOLES/CC)
C      IL AND IR ARE THE STCICHIOMETRIC COEFFICIENTS FOR THE REACTIONS
C                  IL-LEFT SIDE SPECIES/REACTION CORRELATION
C                  IR-RIGHT SIDE SPECIES/REACTION CORRELATION
C                  TP-TRANSLATIONAL/ROTATIONAL TEMPERATURE
C      6 TEMPERATURE EXPANSION PARAMETERS XLGR PER ALOG OF REACTION NR RATE
C         COEFFICIENT RA(NR), 6 TEMPERATURE EXPANSION PARAMETERS XLGK
C         PER SPECIES NS EQUILIBRIUM COEFFICIENT ALOG XLGRP(NS),
C         6 TEMPERATURE EXPANSION PARAMETERS HFX PER SPECIES
C         NS HEAT OF FORMATICN HF(NS) (KCAL/MOLE)
C                  NST-TOTAL SPECIES NUMBER , NRT-TOTAL REACTION NUMBER ***
C      ***** OUTPUT = TEC-CHEMICAL PRODUCTION THERMAL ENERGY (KCAL/CC/SEC)
C                     RCN-CHEMICAL RATE OF FORMATION OF SPECIES  (MOLES/CC/SEC)
C                     RCNT-TCTAL CHEMICAL FORMATION RATE *****
C         *** PRESCRIPTION FOR REACTION NR=
C        PDT(CN(NS)**IL(NS,NR)) - (RA/RV) - PDT(CN(NS)**IR(NS,NR))
C                WHERE PDT-PRODUCT OVER ALL SPECIES NS  *****
      INTEGER RTYP,RSPE
      REAL MWT
      COMMON/RATE/RCON(225,7),WDOT(50),RA(225),IRT(225),
     +IR(50,225),IL(50,225),KR(225,3),KL(225,3),
     +RSPE(225,6),IFLAG(10)
      EQUIVALENCE (IRT,RTYP)
      DIMENSION RTYP(225),RV(225),RP(225),RM(225)
      COMMON/SPECYS/ALPHA(50),G(50)
      COMMON/KON1/CNU(50),NST,NALL,NSPALL,NRT,NT,WE(2),WEXE(2)
     +,MWT(50)
      DATA AVAGAD,R/6.0228E23,1.98717/
      DIMENSION CN(1)
      RTP=R*T
      TPR=T-298.
      CALL MATH(T)
      IF(IFLAG(4).EQ.0)GO TC 1
      WRITE(6,100)
  100 FORMAT(1X,'  J',10X,'RA(J)',15X,'RV(J)')
    1 CONTINUE
      DO 15 J=1,NRT
      YKPT=0.0
      NUL=0
      NUR=0
      DO 5 K=1,3
      KL1= RSPE(J,K)
      IF(KL1.EQ.-1) GO TO 5
      NUL=NUL+KL(J,K)
      YKPT=YKPT-KL(J,K)*G(KL1)
    5 CONTINUE
      DO 10 K=1,3
      KR1=RSPE(J,K+3)
```

```
      IF(KR1.EQ.-1) GO TO 10
      NUR=NUR+KR(J,K)
      YKPT=YKPT+KR(J,K)*G(KR1)
   10 CONTINUE
      INEU=NUL-NUR
C     THE REACTION RATES ARE IN CM**3/(PARTICLE*SECONDS)
      RA(J )=RA(J )*AVAGAD
C     RATES ARE NOW CONVERTED TO CM**3/(MOLE*SECOND)
      RV(J )= RA(J )/EXP(-YKPT/RTP)
C     IF(RCTP(J).EQ.1) RV(J)=0.0
C     NOTE IF RCTP =1 THEN REACTION IS NOT REVERSIBLE
      IF(INEU.NE.0) RV(J )=RV(J )*RTP**INEU
      IF(IFLAG(4).EQ.0)GO TO 15
      WRITE(6,101) J,RA(J),RV(J)
  101 FORMAT(1X,I3,5X,E15.8,5X,E15.8)
   15 CONTINUE
      ISET=1
      IPRINT=1
      IF(IFLAG(5).EQ.0)GO TO 16
      WRITE(6,200)
  200 FORMAT(1X,'  J',10X,'RP(J)',15X,'RM(J)')
   16 CONTINUE
      DO 108 I=1,NST
      WDOT(I)=0.0
      DO 107 J=1,NRT
      IF(ISET.EQ.0) GO TO 25
      RCN1=1.0
      RCN2=1.0
      DO 20 NS1=1,NSPALL
      RCN1=RCN1*CN(NS1)**IL(NS1,J)
      RCN2=RCN2*CN(NS1)**IR(NS1,J)
   20 CONTINUE
      RP(J)=RCN1
      RM(J)=RCN2
      IF(IFLAG(5).EQ.0)GO TO 21
      WRITE(6,201) J,RP(J),RM(J)
  201 FORMAT(1X,I3,5X,E15.8,5X,E15.8)
   21 CONTINUE
   25 CONTINUE
      RKCN1=RP(J)*RA(J)
      RKCN2=RM(J)*RV(J)
      WDOT(I)=WDOT(I)+(IR(I,J)-IL(I,J))*(RKCN1-RKCN2)
  107 CONTINUE
      ISET=0
  108 CONTINUE
      WRITE(6,1016)
 1016 FORMAT(' FINISHED CHMSTY')
      RETURN
      END
      SUBROUTINE MATH(TP)
      INTEGER RTYP,RSPE,REACT,RLP,RRP,SPECIE,SPLP,SPRP
```

```
      COMMON/THERMO/TTB(24),GTB(50,24),CPTB(50,24),HTB(50,24)
      COMMON/RATE/RCON(225,7),WDOT(50,10),RA(225),IRT(225),
     +IR(50,225),IL(50,225),KR(225,3),KL(225,3),
     +RSPE(225,6),IFLAG(10)
      EQUIVALENCE (IRT,RTYP)
      DIMENSION RTYP(1)
      COMMON/SPECYS/ALPHA(50),G(50)
      COMMON/KON1/CNU(50),NST,NALL,NSPALL,NRT,NT,WE(2),WEXE(2)
      DATA JTKEY/1/,R/1.98717/
      P23=2./3.
      JP=JTKEY+1
   10 SDT=TP-TTB(JTKEY)
      HDT=TTB(JP)-TP
      IF(SDT*HDT) 15,52,50
   15 IF(SDT) 30,40,20
C     POSITIVE STEP
   20 JTKEY=JP
      JP=JP+1
      IF(JTKEY-NT) 10,40,40
   30 JP=JTKEY
      JTKEY=JTKEY-1
C     NEGATIVE STEP
      IF(JTKEY.GE.0) GO TO 10
   40 WRITE(6,100) TP,JTKEY
C     OUT OF RANGE
  100 FORMAT(1H ,'   TEMPERATURE OUT OF RANGE-CHEM ',E14.5,I5)
      STOP
   50 SDT=SDT/(SDT*HDT)
      GO TO 54
   52 IF(HDT.EQ.0.)SDT=1.
   54 HDT=1.0-SDT
      DO 60 I=1,NSPALL
      G(I )=GTB(I ,JTKEY)*HDT+GTB(I ,JP)*SDT
   60 CONTINUE
C     RTYP SPECIFIES THE FUNCTION FORM OF THE REACTION RATE. READ IN
C     WHEN RATES ARE READ.
C     THE REACTION RATES ARE IN CM**3/(PARTICLE*SECONDS)
      T13=TP**(-1./3.)
      TP12=SQRT(TP)
      TN12=1./TP12
      TPR=TP*R
C     NOTE THAT WE(1) IS FOR HCL
C     NOTE THE INPUT DATA FOR V,VP,U,UP IS THE FOLLOWING;
C     RTYP=9         V=RCON(J,1)  U=RCON(J,2)
C     RTYP=10        V=RCON(J,1)  VP=RCON(J,2)
C     RTYP=11        U=RCON(J,1)  UP=RCON(J,2)
      DO 300 J=1,NRT
      XLG2=0.0
      NTYP=RTYP(J)
      GO TO(201,202,203,204,205,206,207,
     +208,209,210,211),NTYP
```

```
  201 XLG2=RCON(J ,1)*RCON(J ,3)*EXP(RCON(J ,4)/TP)
C       VT ON HCL BY H ATOMS             RTYP=1
C       XLG2=V*CONT3*EXP(CONT4/T)
        GO TO 250
  202 XLG2=RCON(J ,2)*RCON(J ,3)*EXP(RCON(J ,4)/TP)
C       VT ON H2  BY H ATOMS             RTYP=2
C       XLG2=U*CONT3*EXP(CONT4/T)
        GO TO 250
  203 CONTINUE
        GO TO 250
  204 CONTINUE
C       VT ON H2 BY HCL MOLECULES        RTYP=4
C       VT ON H2 BY AR ATOMS             RTYP=4
C       VT ON H2 BY H2 MOLECULES         RTYP=4
        DE=(WE(2)-2*RCON(J,2)*WEXE(2))
        DE23=DE**P23
        XLG2=RCON(J ,2)*RCON(J ,3)*EXP(RCON(J ,4)*DE23*T13)
C       XLG2=U*CONT3*EXP(CONT4*DE23*T**-.333)
        GO TO 250
  205 CONTINUE
C       VT ON HCL BY H2 MOLECULES        RTYP=5
C       VT ON HCL BY AR ATOMS            RTYP=5
        DE=WE(1)-2*RCON(J,1)*WEXE(1)
        DE23=DE**P23
        XLG2=RCON(J ,1)*(RCON(J ,3)+RCON(J ,5)*EXP(RCON(J ,6)*DE23*T13))
C       DE=WE-2VWEXE
C       XLG2=V*(CONT3+CONT5*EXP(CONT6*DE23*TP**-.333))
        GO TO 250
  206 CONTINUE
        GO TO 250
  207 CONTINUE
C       VT ON HCL BY HCL MOLECULES       RTYP=7
        DE=(WE(1)-2*RCON(J,1)*WEXE(1))
        DE23=DE**P23
        XLG2=RCON(J ,1)*(RCON(J ,3)*EXP(RCON(J ,4)*DE23*T13)+
       +RCON(J ,5)*EXP(RCON(J ,6)*T13))
        GO TO 250
  208 CONTINUE
        GO TO 250
  209 CONTINUE
C       VV ON H2 BY HCL MOLECULES        RTYP=9
C       H2(U)+ HCL(V-1) = H2(U-1)+ HCL(V)
        DE=ABS(WE(2)-2*RCON(J ,2)*WEXE(2)-WE(1)+2*RCON(J ,1)*WEXE(1))
        DE23=DE**P23
        XLG2=RCON(J ,1)*RCON(J ,2)*(RCON(J ,3)+RCON(J ,5)*EXP(RCON(J ,6)*
       1DE23*T13))
C       DE=ABS(WE(2)+2UWEXE(2)-WE(1)-2VWEXE(1))
C       XLG2=V*U*(CONT3+CONT5*EXP(CONT6*DE23*TP**-.333)
        GO TO 250
  210 CONTINUE
C       IV IN HCL                        RTYP=10
```

```
C      HCL(V)+ HCL(VP-1)  = HCL(V-1)+ HCL(VP)
       DE=2*(RCON(J  ,2)-RCON(J  ,1))*WEXE(1)
       DE23=DE**P23
       XLG2=RCON(J  ,1)*RCON(J  ,2)*(RCON(J  ,3)*TN12*EXP(RCON(J  ,4)*DE)+
      1RCON(J  ,5)*TP12*EXP(-(RCON(J  ,6)*DE23+RCON(J  ,7))*T13))
       GO TO 250
   211 CONTINUE
C      IV IN H2                    RTYP=11
C      H2(U)+ H2(UP-1)  = H2(U-1)+ H2(UP)
       DE=2*(RCON(J  ,2)-RCON(J  ,1))*WEXE(2)
       DE23=DE**P23
       XLG2=RCON(J  ,1)*RCON(J  ,2)*(RCON(J  ,3)*TN12*EXP(RCON(J  ,4)*DE)+
      1RCON(J  ,5)*TP12*EXP(-(RCON(J  ,6)*DE23+RCON(J  ,7))*T13))
   250 RA(J)=XLG2
C      WRITE(6,400)   J,T13,DE23,XLG2
   400 FORMAT(1X,I3,E15.8,2X,E15.8,2X,E15.8)
   300 CONTINUE
       RETURN
       END
```

```
C       CONSERVATION OF MASS
      V2=W/(A2*RHO2)
      WRITE(6,50)V2
   50 FORMAT(' V2=',1PE20.8)
C       CHECK CONVERGENCE
      IF(ABS(V2P-V2)/V2.GT.ERR)GO TO 100
      RETURN
  200 WRITE(6,10)T1,T2,P1,P2,V1,V2,Q,W,A2,CP,R
   10 FORMAT(' FLOW SUBROUTINE DID NOT CONVERGE'/(1X,1P6E11.3))
      RETURN 1
      END
      FUNCTION RAD(T,P)
C       THIS FUNCTION IS NOT YET OPERATIONAL
      RAD=110.
      WRITE(6,10)
   10 FORMAT(' FUNCTION RAD IS NOT YET OPERATIONAL, IT RETURNS Q=110.')
      RETURN
      END
```

APPENDIX 5

CHEMISTRY CODE INPUT DATA FOR MODELING THE $HCl-H_2$ SYSTEM

H		1.008	52.103					
	50.	4.968	15.012	-1.232	100.	4.968	21.964	-0.984
	150.	4.968	23.866	-0.736	200.	4.968	25.408	-0.488
	250.	4.968	26.430	-0.244	298.	4.968	27.391	.000
	300.	4.968	27.422	.009	400.	4.968	28.851	0.506
	500.	4.968	29.960	1.003	600.	4.968	30.866	1.500
	700.	4.968	31.631	1.996	800.	4.968	32.295	2.493
	900.	4.968	32.880	2.990	1000.	4.968	33.405	3.487
	1200.	4.968	34.309	4.480	1400.	4.968	35.075	5.474
	1600.	4.968	35.738	6.964	1800.	4.968	36.323	7.461
	2000.	4.968	36.847	8.455	2200.	4.968	37.320	9.448
	2400.	4.968	37.753	10.442	2600.	4.968	38.150	11.435
	2800.	4.968	38.518	12.429	3000.	4.968	38.861	13.423
H2 (	0)	2.016	0.0					
	50.	7.010	18.709	-1.734	100.	6.995	23.567	-1.383
	150.	6.982	26.401	-1.034	200.	6.979	28.409	- .685
	250.	6.979	29.966	-0.336	298.	6.981	31.195	0.000
	300.	6.981	31.238	0.013	400.	6.987	33.248	0.711
	500.	6.995	34.807	1.410	600.	7.010	36.084	2.110
	700.	7.037	37.166	2.813	800.	7.080	38.108	3.518
	900.	7.142	38.946	4.229	1000.	7.219	39.702	4.947
	1200.	7.406	41.034	6.409	1400.	7.612	42.191	7.911
	1600.	7.815	43.221	9.454	1800.	8.005	44.153	11.036
	2000.	8.177	45.005	12.654	2200.	8.330	45.792	14.305
	2400.	8.466	46.522	15.985	2600.	8.588	47.205	17.691
	2800.	8.696	47.854	19.419	3000.	8.794	48.449	21.169

H2 (1)	2.016	11.892					
50.	7.010	18.709	-1.734	100.	6.995	23.567	-1.383
150.	6.982	26.401	-1.034	200.	6.979	28.409	- .685
250.	6.979	29.966	-0.336	298.	6.981	31.195	0.000
300.	6.981	31.238	0.013	400.	6.987	33.248	0.711
500.	6.995	34.807	1.410	600.	7.010	36.084	2.110
700.	7.037	37.166	2.813	800.	7.080	38.108	3.518
900.	7.142	38.946	4.229	1000.	7.219	39.702	4.947
1200.	7.406	41.034	6.409	1400.	7.612	42.191	7.911
1600.	7.815	43.221	9.454	1800.	8.005	44.153	11.036
2000.	8.177	45.005	12.654	2200.	8.330	45.792	14.305
2400.	8.466	46.522	15.985	2600.	8.588	47.205	17.691
2800.	8.696	47.854	19.419	3000.	8.794	48.449	21.169
H2 (2)	2.016	23.110					
50.	7.010	18.709	-1.734	100.	6.995	23.567	-1.383
150.	6.982	26.401	-1.034	200.	6.979	28.409	- .685
250.	6.979	29.966	-0.336	298.	6.981	31.195	0.000
300.	6.981	31.238	0.013	400.	6.987	33.248	0.711
500.	6.995	34.807	1.410	600.	7.010	36.084	2.110
700.	7.037	37.166	2.813	800.	7.080	38.108	3.518
900.	7.142	38.946	4.229	1000.	7.219	39.702	4.947
1200.	7.406	41.034	6.409	1400.	7.612	42.191	7.911
1600.	7.815	43.221	9.454	1800.	8.005	44.153	11.036
2000.	8.177	45.005	12.654	2200.	8.330	45.792	14.305
2400.	8.466	46.522	15.985	2600.	8.588	47.205	17.691
2800.	8.696	47.854	19.419	3000.	8.794	48.449	21.169
H2 (3)	2.016	33.653					
50.	7.010	18.709	-1.734	100.	6.995	23.567	-1.383
150.	6.982	26.401	-1.034	200.	6.979	28.409	- .685
250.	6.979	29.966	-0.336	298.	6.981	31.195	0.000
300.	6.981	31.238	0.013	400.	6.987	33.248	0.711
500.	6.995	34.807	1.410	600.	7.010	36.084	2.110
700.	7.037	37.166	2.813	800.	7.080	38.108	3.518
900.	7.142	38.946	4.229	1000.	7.219	39.702	4.947
1200.	7.406	41.034	6.409	1400.	7.612	42.191	7.911

1600.	7.815	43.221	9.454	1800.	8.005	44.153	11.036
2000.	8.177	45.005	12.654	2200.	8.330	45.792	14.305
2400.	8.466	46.522	15.985	2600.	8.588	47.205	17.691
2800.	8.696	47.854	19.419	3000.	8.794	48.449	21.169
H2 (4)	2.016	43.521					
50.	7.010	18.709	-1.734	100.	6.995	23.567	-1.383
150.	6.982	26.401	-1.034	200.	6.979	28.409	- .685
250.	6.979	29.966	-0.336	298.	6.981	31.195	0.000
300.	6.981	31.238	0.013	400.	6.987	33.248	0.711
500.	6.995	34.807	1.410	600.	7.010	36.084	2.110
700.	7.037	37.166	2.813	800.	7.080	38.108	3.518
900.	7.142	38.946	4.229	1000.	7.219	39.702	4.947
1200.	7.406	41.034	6.409	1400.	7.612	42.191	7.911
1600.	7.815	43.221	9.454	1800.	8.005	44.153	11.036
2000.	8.177	45.005	12.654	2200.	8.330	45.792	14.305
2400.	8.466	46.522	15.985	2600.	8.588	47.205	17.691
2800.	8.696	47.854	19.419	3000.	8.794	48.449	21.169
H2 (5)	2.016	52.714					
50.	7.010	18.709	-1.734	100.	6.995	23.567	-1.383
150.	6.982	26.401	-1.034	200.	6.979	28.409	- .685
250.	6.979	29.966	-0.336	298.	6.981	31.195	0.000
300.	6.981	31.238	0.013	400.	6.987	33.248	0.711
500.	6.995	34.807	1.410	600.	7.010	36.084	2.110
700.	7.037	37.166	2.813	800.	7.080	38.108	3.518
900.	7.142	38.946	4.229	1000.	7.219	39.702	4.947
1200.	7.406	41.034	6.409	1400.	7.612	42.191	7.911
1600.	7.815	43.221	9.454	1800.	8.005	44.153	11.036
2000.	8.177	45.005	12.654	2200.	8.330	45.792	14.305
2400.	8.466	46.522	15.985	2600.	8.588	47.205	17.691
2800.	8.696	47.854	19.419	3000.	8.794	48.449	21.169
H2 (6)	2.016	61.233					
50.	7.010	18.709	-1.734	100.	6.995	23.567	-1.383
150.	6.982	26.401	-1.034	200.	6.979	28.409	- .685
250.	6.979	29.966	-0.336	298.	6.981	31.195	0.000
300.	6.981	31.238	0.013	400.	6.987	33.248	0.711
500.	6.995	34.807	1.410	600.	7.010	36.084	2.110

	700.	7.037	37.166	2.813	800.	7.080	38.108	3.518
	900.	7.142	38.946	4.229	1000.	7.219	39.702	4.947
	1200.	7.406	41.034	6.409	1400.	7.612	42.191	7.911
	1600.	7.815	43.221	9.454	1800.	8.005	44.153	11.036
	2000.	8.177	45.005	12.654	2200.	8.330	45.792	14.305
	2400.	8.466	46.522	15.985	2600.	8.588	47.205	17.691
	2800.	8.696	47.854	19.419	3000.	8.794	48.449	21.169
H2 (	7)	2.016	69.077					
	50.	7.C10	18.709	-1.734	100.	6.995	23.567	-1.383
	150.	6.982	26.401	-1.C34	200.	6.979	28.409	- .685
	250.	6.979	29.966	-0.336	298.	6.981	31.195	0.00C
	300.	6.981	31.238	0.013	400.	6.987	33.248	0.711
	500.	6.995	34.807	1.410	600.	7.010	36.084	2.110
	700.	7.037	37.166	2.813	800.	7.080	38.108	3.518
	900.	7.142	38.946	4.229	1000.	7.219	39.702	4.947
	1200.	7.406	41.034	6.409	1400.	7.612	42.191	7.911
	1600.	7.815	43.221	9.454	1800.	8.005	44.153	11.036
	2000.	8.177	45.005	12.654	2200.	8.330	45.792	14.305
	2400.	8.466	46.522	15.985	2600.	8.588	47.205	17.691
	2800.	8.696	47.854	19.419	3000.	8.794	48.449	21.169
H2 (	8)	2.016	76.247					
	50.	7.010	18.709	-1.734	100.	6.995	23.567	-1.383
	150.	6.982	26.401	-1.034	200.	6.979	28.409	- .685
	250.	6.979	29.966	-0.336	298.	6.981	31.195	0.000
	300.	6.981	31.238	0.013	400.	6.987	33.248	0.711
	500.	6.995	34.807	1.410	600.	7.010	36.084	2.110
	700.	7.037	37.166	2.813	800.	7.080	38.108	3.518
	900.	7.142	38.946	4.229	1000.	7.219	39.702	4.947
	1200.	7.406	41.034	6.409	1400.	7.612	42.191	7.911
	1600.	7.815	43.221	9.454	1800.	8.005	44.153	11.036
	2000.	8.177	45.005	12.654	2200.	8.330	45.792	14.305
	2400.	8.466	46.522	15.985	2600.	8.588	47.205	17.691
	2800.	8.696	47.854	19.419	3000.	8.794	48.449	21.169
HCL(	0)	36.461	-22.063					
	50.	6.961	32.216	-1.727	100.	6.959	37.040	-1.379
	150.	6.960	39.861	-1.031	200.	6.961	41.864	-0.683

250.	6.962	43.417	-0.335	298.	6.964	44.643	.000
300.	6.964	44.687	0.013	400.	6.973	46.691	0.710
500.	7.004	48.249	1.408	600.	7.068	49.532	2.111
700.	7.167	50.628	2.823	800.	7.288	51.593	3.546
900.	7.423	52.459	4.281	1000.	7.560	53.248	5.030
1200.	7.820	54.650	6.569	1400.	8.044	55.873	8.156
1600.	8.231	56.959	9.784	1800.	8.385	57.938	11.446
2000.	8.512	58.828	13.136	2200.	8.618	59.645	14.849
2400.	8.707	60.398	16.582	2600.	8.783	61.098	18.331
2800.	8.849	61.752	20.095	3000.	8.907	62.364	21.870
HCL(1) 36.461		-13.812					
50.	6.961	32.216	-1.727	100.	6.959	37.040	-1.379
150.	6.960	39.861	-1.031	200.	6.961	41.864	-0.683
250.	6.962	43.417	-0.335	298.	6.964	44.643	.000
300.	6.964	44.687	0.013	400.	6.973	46.691	0.710
500.	7.004	48.249	1.408	600.	7.068	49.532	2.111
700.	7.167	50.628	2.823	800.	7.288	51.593	3.546
900.	7.423	52.459	4.281	1000.	7.560	53.248	5.030
1200.	7.820	54.650	6.569	1400.	8.044	55.873	8.156
1600.	8.231	56.959	9.784	1800.	8.385	57.938	11.446
2000.	8.512	58.828	13.136	2200.	8.618	59.645	14.849
2400.	8.707	60.398	16.582	2600.	8.783	61.098	18.331
2800.	8.849	61.752	20.095	3000.	8.907	62.364	21.870
HCL(2) 36.461		- 5.859					
50.	6.961	32.216	-1.727	100.	6.959	37.040	-1.379
150.	6.960	39.861	-1.031	200.	6.961	41.864	-0.683
250.	6.962	43.417	-0.335	298.	6.964	44.643	.000
300.	6.964	44.687	0.013	400.	6.973	46.691	0.710
500.	7.004	48.249	1.408	600.	7.068	49.532	2.111
700.	7.167	50.628	2.823	800.	7.288	51.593	3.546
900.	7.423	52.459	4.281	1000.	7.560	53.248	5.030
1200.	7.820	54.650	6.569	1400.	8.044	55.873	8.156
1600.	8.231	56.959	9.784	1800.	8.385	57.938	11.446
2000.	8.512	58.828	13.136	2200.	8.618	59.645	14.849
2400.	8.707	60.398	16.582	2600.	8.783	61.098	18.331
2800.	8.849	61.752	20.095	3000.	8.907	62.364	21.870

HCL(3)	36.461		1.797					
	50.	6.961	32.216	-1.727	100.	6.959	37.040	-1.379
	150.	6.960	39.861	-1.031	200.	6.961	41.864	-0.683
	250.	6.962	43.417	-0.335	298.	6.964	44.643	.000
	300.	6.964	44.687	0.013	400.	6.973	46.691	0.710
	500.	7.004	48.249	1.408	600.	7.068	49.532	2.111
	700.	7.167	50.628	2.823	800.	7.288	51.593	3.546
	900.	7.423	52.459	4.281	1000.	7.560	53.248	5.030
	1200.	7.820	54.650	6.569	1400.	8.044	55.873	8.156
	1600.	8.231	56.959	9.784	1800.	8.385	57.938	11.446
	2000.	8.512	58.828	13.136	2200.	8.618	59.645	14.849
	2400.	8.707	60.398	16.582	2600.	8.783	61.098	18.331
	2800.	8.849	61.752	20.095	3000.	8.907	62.364	21.870
HCL(4)	36.461		9.155					
	50.	6.961	32.216	-1.727	100.	6.959	37.040	-1.379
	150.	6.960	39.861	-1.031	200.	6.961	41.864	-0.683
	250.	6.962	43.417	-0.335	298.	6.964	44.643	.000
	300.	6.964	44.687	0.013	400.	6.973	46.691	0.710
	500.	7.004	48.249	1.408	600.	7.068	49.532	2.111
	700.	7.167	50.628	2.823	800.	7.288	51.593	3.546
	900.	7.423	52.459	4.281	1000.	7.560	53.248	5.030
	1200.	7.820	54.650	6.569	1400.	8.044	55.873	8.156
	1600.	8.231	56.959	9.784	1800.	8.385	57.938	11.446
	2000.	8.512	58.828	13.136	2200.	8.618	59.645	14.849
	2400.	8.707	60.398	16.582	2600.	8.783	61.098	18.331
	2800.	8.849	61.752	20.095	3000.	8.907	62.364	21.870
HCL(5)	36.461		16.215					
	50.	6.961	32.216	-1.727	100.	6.959	37.040	-1.379
	150.	6.960	39.861	-1.031	200.	6.961	41.864	-0.683
	250.	6.962	43.417	-0.335	298.	6.964	44.643	.000
	300.	6.964	44.687	0.013	400.	6.973	46.691	0.710
	500.	7.004	48.249	1.408	600.	7.068	49.532	2.111
	700.	7.167	50.628	2.823	800.	7.288	51.593	3.546
	900.	7.423	52.459	4.281	1000.	7.560	53.248	5.030
	1200.	7.820	54.650	6.569	1400.	8.044	55.873	8.156
	1600.	8.231	56.959	9.784	1800.	8.385	57.938	11.446

	2000.	8.512	58.828	13.136	2200.	8.618	59.645	14.849
	2400.	8.707	60.398	16.582	2600.	8.783	61.098	18.331
	2800.	8.849	61.752	20.095	3000.	8.907	62.364	21.870
HCL(	6)	36.461	22.978					
	50.	6.961	32.216	-1.727	100.	6.959	37.040	-1.379
	150.	6.960	39.861	-1.031	200.	6.961	41.864	-0.683
	250.	6.962	43.417	-0.335	298.	6.964	44.643	.000
	300.	6.964	44.687	0.013	400.	6.973	46.691	0.710
	500.	7.004	48.249	1.408	600.	7.068	49.532	2.111
	700.	7.167	50.628	2.823	800.	7.288	51.593	3.546
	900.	7.423	52.459	4.281	1000.	7.560	53.248	5.030
	1200.	7.820	54.650	6.569	1400.	8.044	55.873	8.156
	1600.	8.231	56.959	9.784	1800.	8.385	57.938	11.446
	2000.	8.512	58.828	13.136	2200.	8.618	59.645	14.849
	2400.	8.707	60.398	16.582	2600.	8.783	61.098	18.331
	2800.	8.849	61.752	20.095	3000.	8.907	62.364	21.870
HCL(	7)	36.461	29.442					
	50.	6.961	32.216	-1.727	100.	6.959	37.040	-1.379
	150.	6.960	39.861	-1.031	200.	6.961	41.864	-0.683
	250.	6.962	43.417	-0.335	298.	6.964	44.643	.000
	300.	6.964	44.687	0.013	400.	6.973	46.691	0.710
	500.	7.004	48.249	1.408	600.	7.068	49.532	2.111
	700.	7.167	50.628	2.823	800.	7.288	51.593	3.546
	900.	7.423	52.459	4.281	1000.	7.560	53.248	5.030
	1200.	7.820	54.650	6.569	1400.	8.044	55.873	8.156
	1600.	8.231	56.959	9.784	1800.	8.385	57.938	11.446
	2000.	8.512	58.828	13.136	2200.	8.618	59.645	14.849
	2400.	8.707	60.398	16.582	2600.	8.783	61.098	18.331
	2800.	8.849	61.752	20.095	3000.	8.907	62.364	21.870
HCL(	8)	36.461	36.610					
	50.	6.961	32.216	-1.727	100.	6.959	37.040	-1.379
	150.	6.960	39.861	-1.031	200.	6.961	41.864	-0.683
	250.	6.962	43.417	-0.335	298.	6.964	44.643	.000
	300.	6.964	44.687	0.013	400.	6.973	46.691	0.710
	500.	7.004	48.249	1.408	600.	7.068	49.532	2.111
	700.	7.167	50.628	2.823	800.	7.288	51.593	3.546

	900.	7.423	52.459	4.281	1000.	7.560	53.248	5.030
	1200.	7.820	54.650	6.569	1400.	8.044	55.873	8.156
	1600.	8.231	56.959	9.784	1800.	8.385	57.938	11.446
	2000.	8.512	58.828	13.136	2200.	8.618	59.645	14.849
	2400.	8.707	60.398	16.582	2600.	8.783	61.098	18.331
	2800.	8.849	61.752	20.095	3000.	8.907	62.364	21.870
HCL(9)		36.461	41.479					
	50.	6.961	32.216	-1.727	100.	6.959	37.040	-1.379
	150.	6.960	39.861	-1.031	200.	6.961	41.864	-0.683
	250.	6.962	43.417	-0.335	298.	6.964	44.643	.000
	300.	6.964	44.687	0.013	400.	6.973	46.691	0.710
	500.	7.004	48.249	1.408	600.	7.068	49.532	2.111
	700.	7.167	50.628	2.823	800.	7.288	51.593	3.546
	900.	7.423	52.459	4.281	1000.	7.560	53.248	5.030
	1200.	7.820	54.650	6.569	1400.	8.044	55.873	8.156
	1600.	8.231	56.959	9.784	1800.	8.385	57.938	11.446
	2000.	8.512	58.828	13.136	2200.	8.618	59.645	14.849
	2400.	8.707	60.398	16.582	2600.	8.783	61.098	18.331
	2800.	8.849	61.752	20.095	3000.	8.907	62.364	21.870
HCL(10)		36.461	47.052					
	50.	6.961	32.216	-1.727	100.	6.959	37.040	-1.379
	150.	6.960	39.861	-1.031	200.	6.961	41.864	-0.683
	250.	6.962	43.417	-0.335	298.	6.964	44.643	.000
	300.	6.964	44.687	0.013	400.	6.973	46.691	0.710
	500.	7.004	48.249	1.408	600.	7.068	49.532	2.111
	700.	7.167	50.628	2.823	800.	7.288	51.593	3.546
	900.	7.423	52.459	4.281	1000.	7.560	53.248	5.030
	1200.	7.820	54.650	6.569	1400.	8.044	55.873	8.156
	1600.	8.231	56.959	9.784	1800.	8.385	57.938	11.446
	2000.	8.512	58.828	13.136	2200.	8.618	59.645	14.849
	2400.	8.707	60.398	16.582	2600.	8.783	61.098	18.331
	2800.	8.849	61.752	20.095	3000.	8.907	62.364	21.870
AR		39.948	0.0					
	50.	4.968	30.010	-1.481	100.	4.968	31.554	-0.984
	150.	4.968	33.569	-0.736	200.	4.968	34.998	-0.488
	250.	4.968	36.106	-0.239	298.	4.968	36.981	0.000

300.	4.968	37.012	0.009	400.	4.968	38.441	0.506
500.	4.968	39.550	1.003	600.	4.968	40.456	1.500
700.	4.968	41.221	1.996	800.	4.968	41.885	2.493
900.	4.968	42.470	2.990	1000.	4.968	42.993	3.487
1200.	4.968	43.899	4.480	1400.	4.968	44.665	5.474
1600.	4.968	45.328	6.467	1800.	4.968	45.913	7.461
2000.	4.968	46.437	8.455	2200.	4.968	46.910	9.448
2400.	4.968	47.343	10.442	2600.	4.968	47.740	11.435
2800.	4.968	48.108	12.429	3000.	4.968	48.451	13.423
H2 (999)	2.016	0.0					
50.	7.010	18.709	-1.734	100.	6.995	23.567	-1.383
150.	6.982	26.401	-1.034	200.	6.979	28.409	- .685
250.	6.979	29.966	-0.336	298.	6.981	31.195	0.000
300.	6.981	31.238	0.013	400.	6.987	33.248	0.711
500.	6.995	34.807	1.410	600.	7.010	36.084	2.110
700.	7.037	37.166	2.813	800.	7.080	38.108	3.518
900.	7.142	38.946	4.229	1000.	7.219	39.702	4.947
1200.	7.406	41.034	6.409	1400.	7.612	42.191	7.911
1600.	7.815	43.221	9.454	1800.	8.005	44.153	11.036
2000.	8.177	45.005	12.654	2200.	8.330	45.792	14.305
2400.	8.466	46.522	15.985	2600.	8.588	47.205	17.691
2800.	8.696	47.854	19.419	3000.	8.794	48.449	21.169
HCL(999)	36.461	-22.063					
50.	6.961	32.216	-1.727	100.	6.959	37.040	-1.379
150.	6.960	39.861	-1.031	200.	6.961	41.864	-0.683
250.	6.962	43.417	-0.335	298.	6.964	44.643	.000
300.	6.964	44.687	0.013	400.	6.973	46.691	0.710
500.	7.004	48.249	1.408	600.	7.068	49.532	2.111
700.	7.167	50.628	2.823	800.	7.298	51.593	3.546
900.	7.423	52.459	4.281	1000.	7.560	53.248	5.030
1200.	7.820	54.650	6.569	1400.	8.044	55.873	8.156
1600.	8.231	56.959	9.784	1800.	8.385	57.938	11.446
2000.	8.512	58.828	13.136	2200.	8.618	59.645	14.849
2400.	8.707	60.398	16.582	2600.	8.783	61.098	18.331
2800.	8.849	61.752	20.095	3000.	8.907	62.364	21.870

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1HCL(  1)+1HCL(999)+          =1HCL(  0)+1HCL(999)+
1 7  1.                          4.676E-10      -.379  3.130E-16      27.91
1HCL(  2)+1HCL(999)+          =1HCL(  1)+1HCL(999)+
1 7  2.                          4.676E-10      -.379  3.130E-16      27.91
1HCL(  3)+1HCL(999)+          =1HCL(  2)+1HCL(999)+
1 7  3.                          4.676E-10      -.379  3.130E-16      27.91
1HCL(  4)+1HCL(999)+          =1HCL(  3)+1HCL(999)+
1 7  4.                          4.676E-10      -.379  3.130E-16      27.91
1HCL(  5)+1HCL(999)+          =1HCL(  4)+1HCL(999)+
1 7  5.                          4.676E-10      -.379  3.130E-16      27.91
1HCL(  6)+1HCL(999)+          =1HCL(  5)+1HCL(999)+
1 7  6.                          4.676E-10      -.379  3.130E-16      27.91
1HCL(  7)+1HCL(999)+          =1HCL(  6)+1HCL(999)+
1 7  7.                          4.676E-10      -.379  3.130E-16      27.91
1HCL(  8)+1HCL(999)+          =1HCL(  7)+1HCL(999)+
1 7  8.                          4.676E-10      -.379  3.130E-16      27.91
1HCL(  9)+1HCL(999)+          =1HCL(  8)+1HCL(999)+
1 7  9.                          4.676E-10      -.379  3.130E-16      27.91
1HCL( 10)+1HCL(999)+          =1HCL(  9)+1HCL(999)+
1 7 10.                          4.676E-10      -.379  3.130E-16      27.91
1HCL(  1)+1H2  (999)+         =1HCL(  0)+1H2  (999)+
1 5  1.                            2.98E-15             5.23E-10     -.4037
1HCL(  2)+1H2  (999)+         =1HCL(  1)+1H2  (999)+
1 5  2.                            2.98E-15             5.23E-10     -.4037
1HCL(  3)+1H2  (999)+         =1HCL(  2)+1H2  (999)+
1 5  3.                            2.98E-15             5.23E-10     -.4037
1HCL(  4)+1H2  (999)+         =1HCL(  3)+1H2  (999)+
1 5  4.                            2.98E-15             5.23E-10     -.4037
1HCL(  5)+1H2  (999)+         =1HCL(  4)+1H2  (999)+
1 5  5.                            2.98E-15             5.23E-10     -.4037
1HCL(  6)+1H2  (999)+         =1HCL(  5)+1H2  (999)+
1 5  6.                            2.98E-15             5.23E-10     -.4037
1HCL(  7)+1H2  (999)+         =1HCL(  6)+1H2  (999)+
1 5  7.                            2.98E-15             5.23E-10     -.4037
1HCL(  8)+1H2  (999)+         =1HCL(  7)+1H2  (999)+
1 5  8.                            2.98E-15             5.23E-10     -.4037
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1HCL(  9)+1H2  (999)+          =1HCL(  8)+1H2  (999)+
1 5  9.                            2.98E-15                 5.23E-10     -.4037
1HCL( 10)+1H2  (999)+          =1HCL(  9)+1H2  (999)+
1 5 10.                            2.98E-15                 5.23E-10     -.4037
1HCL(  1)+1H           +       =1HCL(  0)+1H          +
1 1  1.                            3.70E-11      -500.
1HCL(  2)+1H           +       =1HCL(  1)+1H          +
1 1  2.                            3.70E-11      -500.
1HCL(  3)+1H           +       =1HCL(  2)+1H          +
1 1  3.                            3.70E-11      -500.
1HCL(  4)+1H           +       =1HCL(  3)+1H          +
1 1  4.                            3.70E-11      -500.
1HCL(  5)+1H           +       =1HCL(  4)+1H          +
1 1  5.                            3.70E-11      -500.
1HCL(  6)+1H           +       =1HCL(  5)+1H          +
1 1  6.                            3.70E-11      -500.
1HCL(  7)+1H           +       =1HCL(  6)+1H          +
1 1  7.                            3.70E-11      -500.
1HCL(  8)+1H           +       =1HCL(  7)+1H          +
1 1  8.                            3.70E-11      -500.
1HCL(  9)+1H           +       =1HCL(  8)+1H          +
1 1  9.                            3.70E-11      -500.
1HCL( 10)+1H           +       =1HCL(  9)+1H          +
1 1 10.                            3.70E-11      -500.
1HCL(  1)+1AR          +       =1HCL(  0)+1AR         +
1 5  1.                            3.00E-19                 3.49E- 8      -.896
1HCL(  2)+1AR          +       =1HCL(  1)+1AR         +
1 5  2.                            3.00E-19                 3.49E- 8      -.896
1HCL(  3)+1AR          +       =1HCL(  2)+1AR         +
1 5  3.                            3.00E-19                 3.49E- 8      -.896
1HCL(  4)+1AR          +       =1HCL(  3)+1AR         +
1 5  4.                            3.00E-19                 3.49E- 8      -.896
1HCL(  5)+1AR          +       =1HCL(  4)+1AR         +
1 5  5.                            3.00E-19                 3.49E- 8      -.896
1HCL(  6)+1AR          +       =1HCL(  5)+1AR         +
1 5  6.                            3.00E-19                 3.49E- 8      -.896
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1HCL(  7)+1AR          +    =1HCL(  6)+1AR          +
1 5  7.                       3.00E-19                 3.49E- 8     -.896
1HCL(  8)+1AR          +    =1HCL(  7)+1AR          +
1 5  8.                       3.00E-19                 3.49E- 8     -.896
1HCL(  9)+1AR          +    =1HCL(  8)+1AR          +
1 5  9.                       3.00E-19                 3.49E- 8     -.896
1HCL( 10)+1AR          +    =1HCL(  9)+1AR          +
1 5 10.                       3.00E-19                 3.49E- 8     -.896
1H2 (  1)+1H2  (999)+       =1H2 (  0)+1H2  (999)+
1 4      1.                  2.177E- 9    -.4443
1H2 (  2)+1H2  (999)+       =1H2 (  1)+1H2  (999)+
1 4      2.                  2.177E- 9    -.4443
1H2 (  3)+1H2  (999)+       =1H2 (  2)+1H2  (999)+
1 4      3.                  2.177E- 9    -.4443
1H2 (  4)+1H2  (999)+       =1H2 (  3)+1H2  (999)+
1 4      4.                  2.177E- 9    -.4443
1H2 (  5)+1H2  (999)+       =1H2 (  4)+1H2  (999)+
1 4      5.                  2.177E- 9    -.4443
1H2 (  6)+1H2  (999)+       =1H2 (  5)+1H2  (999)+
1 4      6.                  2.177E- 9    -.4443
1H2 (  7)+1H2  (999)+       =1H2 (  6)+1H2  (999)+
1 4      7.                  2.177E- 9    -.4443
1H2 (  8)+1H2  (999)+       =1H2 (  7)+1H2  (999)+
1 4      8.                  2.177E- 9    -.4443
1H2 (  1)+1HCL(999)+        =1H2 (  0)+1HCL(999)+
1 4      1.                  4.354E-10    -.4443
1H2 (  2)+1HCL(999)+        =1H2 (  1)+1HCL(999)+
1 4      2.                  4.354E-10    -.4443
1H2 (  3)+1HCL(999)+        =1H2 (  2)+1HCL(999)+
1 4      3.                  4.354E-10    -.4443
1H2 (  4)+1HCL(999)+        =1H2 (  3)+1HCL(999)+
1 4      4.                  4.354E-10    -.4443
1H2 (  5)+1HCL(999)+        =1H2 (  4)+1HCL(999)+
1 4      5.                  4.354E-10    -.4443
1H2 (  6)+1HCL(999)+        =1H2 (  5)+1HCL(999)+
1 4      6.                  4.354E-10    -.4443
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1H2  (   7)+1HCL(999)+          =1H2  (   6)+1HCL(999)+
1 4      7.                        4.354E-10      -.4443
1H2  (   8)+1HCL(999)+          =1H2  (   7)+1HCL(999)+
1 4      8.                        4.354E-10      -.4443
1H2  (   1)+1H                  =1H2  (   0)+1H         +
1 2      1.                        1.71E-12       -500.
1H2  (   2)+1H                  =1H2  (   1)+1H         +
1 2      2.                        1.71E-12       -500.
1H2  (   3)+1H                  =1H2  (   2)+1H         +
1 2      3.                        1.71E-12       -500.
1H2  (   4)+1H                  =1H2  (   3)+1H         +
1 2      4.                        1.71E-12       -500.
1H2  (   5)+1H                  =1H2  (   4)+1H         +
1 2      5.                        1.71E-12       -500.
1H2  (   6)+1H                  =1H2  (   5)+1H         +
1 2      6.                        1.71E-12       -500.
1H2  (   7)+1H                  =1H2  (   6)+1H         +
1 2      7.                        1.71E-12       -500.
1H2  (   8)+1H                  =1H2  (   7)+1H         +
1 2      8.                        1.71E-12       -500.
1H2  (   1)+1AR                 =1H2  (   0)+1AR        +
1 4      1.                        5.44E-10       -.4443
1H2  (   2)+1AR                 =1H2  (   1)+1AR        +
1 4      2.                        5.44E-10       -.4443
1H2  (   3)+1AR                 =1H2  (   2)+1AR        +
1 4      3.                        5.44E-10       -.4443
1H2  (   4)+1AR                 =1H2  (   3)+1AR        +
1 4      4.                        5.44E-10       -.4443
1H2  (   5)+1AR                 =1H2  (   4)+1AR        +
1 4      5.                        5.44E-10       -.4443
1H2  (   6)+1AR                 =1H2  (   5)+1AR        +
1 4      6.                        5.44E-10       -.4443
1H2  (   7)+1AR                 =1H2  (   6)+1AR        +
1 4      7.                        5.44E-10       -.4443
1H2  (   8)+1AR                 =1H2  (   7)+1AR        +
1 4      8.                        5.44E-10       -.4443
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```
1HCL(  0)+1H2  (  1)+          =1HCL(  1)+1H2  (  0)+
1 9  1. 1.                          5.3E-14              4.98E-10     -.6299
1HCL(  1)+1H2  (  1)+          =1HCL(  2)+1H2  (  0)+
1 9  2. 1.                          5.3E-14              4.98E-10     -.6299
1HCL(  2)+1H2  (  1)+          =1HCL(  3)+1H2  (  0)+
1 9  3. 1.                          5.3E-14              4.98E-10     -.6299
1HCL(  3)+1H2  (  1)+          =1HCL(  4)+1H2  (  0)+
1 9  4. 1.                          5.3E-14              4.98E-10     -.6299
1HCL(  4)+1H2  (  1)+          =1HCL(  5)+1H2  (  0)+
1 9  5. 1.                          5.3E-14              4.98E-10     -.6299
1HCL(  5)+1H2  (  1)+          =1HCL(  6)+1H2  (  0)+
1 9  6. 1.                          5.3E-14              4.98E-10     -.6299
1HCL(  6)+1H2  (  1)+          =1HCL(  7)+1H2  (  0)+
1 9  7. 1.                          5.3E-14              4.98E-10     -.6299
1HCL(  7)+1H2  (  1)+          =1HCL(  8)+1H2  (  0)+
1 9  8. 1.                          5.3E-14              4.98E-10     -.6299
1HCL(  8)+1H2  (  1)+          =1HCL(  9)+1H2  (  0)+
1 9  9. 1.                          5.3E-14              4.98E-10     -.6299
1HCL(  9)+1H2  (  1)+          =1HCL( 10)+1H2  (  0)+
1 9 10. 1.                          5.3E-14              4.98E-10     -.6299
1HCL(  0)+1H2  (  2)+          =1HCL(  1)+1H2  (  1)+
1 9  1. 2.                          5.3E-14              4.98E-10     -.6299
1HCL(  1)+1H2  (  2)+          =1HCL(  2)+1H2  (  1)+
1 9  2. 2.                          5.3E-14              4.98E-10     -.6299
1HCL(  2)+1H2  (  2)+          =1HCL(  3)+1H2  (  1)+
1 9  3. 2.                          5.3E-14              4.98E-10     -.6299
1HCL(  3)+1H2  (  2)+          =1HCL(  4)+1H2  (  1)+
1 9  4. 2.                          5.3E-14              4.98E-10     -.6299
1HCL(  4)+1H2  (  2)+          =1HCL(  5)+1H2  (  1)+
1 9  5. 2.                          5.3E-14              4.98E-10     -.6299
1HCL(  5)+1H2  (  2)+          =1HCL(  6)+1H2  (  1)+
1 9  6. 2.                          5.3E-14              4.98E-10     -.6299
1HCL(  6)+1H2  (  2)+          =1HCL(  7)+1H2  (  1)+
1 9  7. 2.                          5.3E-14              4.98E-10     -.6299
1HCL(  7)+1H2  (  2)+          =1HCL(  8)+1H2  (  1)+
1 9  8. 2.                          5.3E-14              4.98E-10     -.6299
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1HCL(  8)+1H2  (  2)+        =1HCL(  9)+1H2  (  1)+
1 9  9. 2.                       5.3E-14             4.98E-10    -.6299
1HCL(  9)+1H2  (  2)+        =1HCL( 10)+1H2  (  1)+
1 9 10. 2.                       5.3E-14             4.98E-10    -.6299
1HCL(  0)+1H2  (  3)+        =1HCL(  1)+1H2  (  2)+
1 9  1. 3.                       5.3E-14             4.98E-10    -.6299
1HCL(  1)+1H2  (  3)+        =1HCL(  2)+1H2  (  2)+
1 9  2. 3.                       5.3E-14             4.98E-10    -.6299
1HCL(  2)+1H2  (  3)+        =1HCL(  3)+1H2  (  2)+
1 9  3. 3.                       5.3E-14             4.98E-10    -.6299
1HCL(  3)+1H2  (  3)+        =1HCL(  4)+1H2  (  2)+
1 9  4. 3.                       5.3E-14             4.98E-10    -.6299
1HCL(  4)+1H2  (  3)+        =1HCL(  5)+1H2  (  2)+
1 9  5. 3.                       5.3E-14             4.98E-10    -.6299
1HCL(  5)+1H2  (  3)+        =1HCL(  6)+1H2  (  2)+
1 9  6. 3.                       5.3E-14             4.98E-10    -.6299
1HCL(  6)+1H2  (  3)+        =1HCL(  7)+1H2  (  2)+
1 9  7. 3.                       5.3E-14             4.98E-10    -.6299
1HCL(  7)+1H2  (  3)+        =1HCL(  8)+1H2  (  2)+
1 9  8. 3.                       5.3E-14             4.98E-10    -.6299
1HCL(  8)+1H2  (  3)+        =1HCL(  9)+1H2  (  2)+
1 9  9. 3.                       5.3E-14             4.98E-10    -.6299
1HCL(  9)+1H2  (  3)+        =1HCL( 10)+1H2  (  2)+
1 9 10. 3.                       5.3E-14             4.98E-10    -.6299
1HCL(  0)+1H2  (  4)+        =1HCL(  1)+1H2  (  3)+
1 9  1. 4.                       5.3E-14             4.98E-10    -.6299
1HCL(  1)+1H2  (  4)+        =1HCL(  2)+1H2  (  3)+
1 9  2. 4.                       5.3E-14             4.98E-10    -.6299
1HCL(  2)+1H2  (  4)+        =1HCL(  3)+1H2  (  3)+
1 9  3. 4.                       5.3E-14             4.98E-10    -.6299
1HCL(  3)+1H2  (  4)+        =1HCL(  4)+1H2  (  3)+
1 9  4. 4.                       5.3E-14             4.98E-10    -.6299
1HCL(  4)+1H2  (  4)+        =1HCL(  5)+1H2  (  3)+
1 9  5. 4.                       5.3E-14             4.98E-10    -.6299
1HCL(  5)+1H2  (  4)+        =1HCL(  6)+1H2  (  3)+
1 9  6. 4.                       5.3E-14             4.98E-10    -.6299
```

```
1HCL(  6)+1H2  (  4)+          =1HCL(  7)+1H2  (  3)+
1 9  7. 4.                          5.3E-14          4.98E-10   -.6299
1HCL(  7)+1H2  (  4)+          =1HCL(  8)+1H2  (  3)+
1 9  8. 4.                          5.3E-14          4.98E-10   -.6299
1HCL(  8)+1H2  (  4)+          =1HCL(  9)+1H2  (  3)+
1 9  9. 4.                          5.3E-14          4.98E-10   -.6299
1HCL(  9)+1H2  (  4)+          =1HCL( 10)+1H2  (  3)+
1 9 10. 4.                          5.3E-14          4.98E-10   -.6299
1HCL(  0)+1H2  (  5)+          =1HCL(  1)+1H2  (  4)+
1 9  1. 5.                          5.3E-14          4.98E-10   -.6299
1HCL(  1)+1H2  (  5)+          =1HCL(  2)+1H2  (  4)+
1 9  2. 5.                          5.3E-14          4.98E-10   -.6299
1HCL(  2)+1H2  (  5)+          =1HCL(  3)+1H2  (  4)+
1 9  3. 5.                          5.3E-14          4.98E-10   -.6299
1HCL(  3)+1H2  (  5)+          =1HCL(  4)+1H2  (  4)+
1 9  4. 5.                          5.3E-14          4.98E-10   -.6299
1HCL(  4)+1H2  (  5)+          =1HCL(  5)+1H2  (  4)+
1 9  5. 5.                          5.3E-14          4.98E-10   -.6299
1HCL(  5)+1H2  (  5)+          =1HCL(  6)+1H2  (  4)+
1 9  6. 5.                          5.3E-14          4.98E-10   -.6299
1HCL(  6)+1H2  (  5)+          =1HCL(  7)+1H2  (  4)+
1 9  7. 5.                          5.3E-14          4.98E-10   -.6299
1HCL(  7)+1H2  (  5)+          =1HCL(  8)+1H2  (  4)+
1 9  8. 5.                          5.3E-14          4.98E-10   -.6299
1HCL(  8)+1H2  (  5)+          =1HCL(  9)+1H2  (  4)+
1 9  9. 5.                          5.3E-14          4.98E-10   -.6299
1HCL(  9)+1H2  (  5)+          =1HCL( 10)+1H2  (  4)+
1 9 10. 5.                          5.3E-14          4.98E-10   -.6299
1HCL(  0)+1H2  (  6)+          =1HCL(  1)+1H2  (  5)+
1 9  1. 6.                          5.3E-14          4.98E-10   -.6299
1HCL(  1)+1H2  (  6)+          =1HCL(  2)+1H2  (  5)+
1 9  2. 6.                          5.3E-14          4.98E-10   -.6299
1HCL(  2)+1H2  (  6)+          =1HCL(  3)+1H2  (  5)+
1 9  3. 6.                          5.3E-14          4.98E-10   -.6299
1HCL(  3)+1H2  (  6)+          =1HCL(  4)+1H2  (  5)+
1 9  4. 6.                          5.3E-14          4.98E-10   -.6299
```

```
1HCL(  4)+1H2  (  6)+          =1HCL(  5)+1H2  (  5)+
1 9  5. 6.                         5.3E-14              4.98E-10    -.6299
1HCL(  5)+1H2  (  6)+          =1HCL(  6)+1H2  (  5)+
1 9  6. 6.                         5.3E-14              4.98E-10    -.6299
1HCL(  6)+1H2  (  6)+          =1HCL(  7)+1H2  (  5)+
1 9  7. 6.                         5.3E-14              4.98E-10    -.6299
1HCL(  7)+1H2  (  6)+          =1HCL(  8)+1H2  (  5)+
1 9  8. 6.                         5.3E-14              4.98E-10    -.6299
1HCL(  8)+1H2  (  6)+          =1HCL(  9)+1H2  (  5)+
1 9  9. 6.                         5.3E-14              4.98E-10    -.6299
1HCL(  9)+1H2  (  6)+          =1HCL( 10)+1H2  (  5)+
1 9 10. 6.                         5.3E-14              4.98E-10    -.6299
1HCL(  0)+1H2  (  7)+          =1HCL(  1)+1H2  (  6)+
1 9  1. 7.                         5.3E-14              4.98E-10    -.6299
1HCL(  1)+1H2  (  7)+          =1HCL(  2)+1H2  (  6)+
1 9  2. 7.                         5.3E-14              4.98E-10    -.6299
1HCL(  2)+1H2  (  7)+          =1HCL(  3)+1H2  (  6)+
1 9  3. 7.                         5.3E-14              4.98E-10    -.6299
1HCL(  3)+1H2  (  7)+          =1HCL(  4)+1H2  (  6)+
1 9  4. 7.                         5.3E-14              4.98E-10    -.6299
1HCL(  4)+1H2  (  7)+          =1HCL(  5)+1H2  (  6)+
1 9  5. 7.                         5.3E-14              4.98E-10    -.6299
1HCL(  5)+1H2  (  7)+          =1HCL(  6)+1H2  (  6)+
1 9  6. 7.                         5.3E-14              4.98E-10    -.6299
1HCL(  6)+1H2  (  7)+          =1HCL(  7)+1H2  (  6)+
1 9  7. 7.                         5.3E-14              4.98E-10    -.6299
1HCL(  7)+1H2  (  7)+          =1HCL(  8)+1H2  (  6)+
1 9  8. 7.                         5.3E-14              4.98E-10    -.6299
1HCL(  8)+1H2  (  7)+          =1HCL(  9)+1H2  (  6)+
1 9  9. 7.                         5.3E-14              4.98E-10    -.6299
1HCL(  9)+1H2  (  7)+          =1HCL( 10)+1H2  (  6)+
1 9 10. 7.                         5.3E-14              4.98E-10    -.6299
1HCL(  0)+1H2  (  8)+          =1HCL(  1)+1H2  (  7)+
1 9  1. 8.                         5.3E-14              4.98E-10    -.6299
1HCL(  1)+1H2  (  8)+          =1HCL(  2)+1H2  (  7)+
1 9  2. 8.                         5.3E-14              4.98E-10    -.6299
```

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1HCL(  2)+1H2  (  8)+        =1HCL(  3)+1H2  (  7)+
1 9  3. 8.                      5.3E-14            4.98E-10     -.6299
1HCL(  3)+1H2  (  8)+        =1HCL(  4)+1H2  (  7)+
1 9  4. 8.                      5.3E-14            4.98E-10     -.6299
1HCL(  4)+1H2  (  8)+        =1HCL(  5)+1H2  (  7)+
1 9  5. 8.                      5.3E-14            4.98E-10     -.6299
1HCL(  5)+1H2  (  8)+        =1HCL(  6)+1H2  (  7)+
1 9  6. 8.                      5.3E-14            4.98E-10     -.6299
1HCL(  6)+1H2  (  8)+        =1HCL(  7)+1H2  (  7)+
1 9  7. 8.                      5.3E-14            4.98E-10     -.6299
1HCL(  7)+1H2  (  8)+        =1HCL(  8)+1H2  (  7)+
1 9  8. 8.                      5.3E-14            4.98E-10     -.6299
1HCL(  8)+1H2  (  8)+        =1HCL(  9)+1H2  (  7)+
1 9  9. 8.                      5.3E-14            4.98E-10     -.6299
1HCL(  9)+1H2  (  8)+        =1HCL( 10)+1H2  (  7)+
1 9 10. 8.                      5.3E-14            4.98E-10     -.6299
2HCL(  1)+                   =1HCL(  0)+1HCL(  2)
110  1. 2.                    6.769E-11-4.638E- 3 1.941E-12      0.495      40.246
1HCL(  1)+1HCL(  2)+         =1HCL(  0)+1HCL(  3)
110  1. 3.                    6.769E-11-4.638E- 3 1.941E-12      0.495      40.246
1HCL(  1)+1HCL(  3)+         =1HCL(  0)+1HCL(  4)
110  1. 4.                    6.769E-11-4.638E- 3 1.941E-12      0.495      40.246
1HCL(  1)+1HCL(  4)+         =1HCL(  0)+1HCL(  5)
110  1. 5.                    6.769E-11-4.638E- 3 1.941E-12      0.495      40.246
1HCL(  1)+1HCL(  5)+         =1HCL(  0)+1HCL(  6)
110  1. 6.                    6.769E-11-4.638E- 3 1.941E-12      0.495      40.246
1HCL(  1)+1HCL(  6)+         =1HCL(  0)+1HCL(  7)
110  1. 7.                    6.769E-11-4.638E- 3 1.941E-12      0.495      40.246
1HCL(  1)+1HCL(  7)+         =1HCL(  0)+1HCL(  8)
110  1. 8.                    6.769E-11-4.638E- 3 1.941E-12      0.495      40.246
1HCL(  1)+1HCL(  8)+         =1HCL(  0)+1HCL(  9)
110  1. 9.                    6.769E-11-4.638E- 3 1.941E-12      0.495      40.246
1HCL(  1)+1HCL(  9)+         =1HCL(  0)+1HCL( 10)
110  1.10.                    6.769E-11-4.638E- 3 1.941E-12      0.495      40.246
2HCL(  2)+                   =1HCL(  1)+1HCL(  3)
110  2. 3.                    6.769E-11-4.638E- 3 1.941E-12      0.495      40.246
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1HCL(  2)+1HCL(  3)+       =1HCL(  1)+1HCL(  4)
110   2. 4.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
1HCL(  2)+1HCL(  4)+       =1HCL(  1)+1HCL(  5)
110   2. 5.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
1HCL(  2)+1HCL(  5)+       =1HCL(  1)+1HCL(  6)
110   2. 6.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
1HCL(  2)+1HCL(  6)+       =1HCL(  1)+1HCL(  7)
110   2. 7.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
1HCL(  2)+1HCL(  7)+       =1HCL(  1)+1HCL(  8)
110   2. 8.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
1HCL(  2)+1HCL(  8)+       =1HCL(  1)+1HCL(  9)
110   2. 9.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
1HCL(  2)+1HCL(  9)+       =1HCL(  1)+1HCL( 10)
110   2.10.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
2HCL(  3)+                 =1HCL(  2)+1HCL(  4)
110   3. 4.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
1HCL(  3)+1HCL(  4)+       =1HCL(  2)+1HCL(  5)
110   3. 5.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
1HCL(  3)+1HCL(  5)+       =1HCL(  2)+1HCL(  6)
110   3. 6.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
1HCL(  3)+1HCL(  6)+       =1HCL(  2)+1HCL(  7)
110   3. 7.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
1HCL(  3)+1HCL(  7)+       =1HCL(  2)+1HCL(  8)
110   3. 8.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
1HCL(  3)+1HCL(  8)+       =1HCL(  2)+1HCL(  9)
110   3. 9.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
1HCL(  3)+1HCL(  9)+       =1HCL(  2)+1HCL( 10)
110   3.10.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
2HCL(  4)+                 =1HCL(  3)+1HCL(  5)
110   4. 5.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
1HCL(  4)+1HCL(  5)        =1HCL(  3)+1HCL(  6)
110   4. 6.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
1HCL(  4)+1HCL(  6)        =1HCL(  3)+1HCL(  7)
110   4. 7.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
1HCL(  4)+1HCL(  7)        =1HCL(  3)+1HCL(  8)
110   4. 8.                  6.769E-11-4.638E- 3 1.941E-12    0.495    40.246
```

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1HCL(  4)+1HCL(  8)          =1HCL(  3)+1HCL(  9)
110  4. 9.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
1HCL(  4)+1HCL(  9)          =1HCL(  3)+1HCL( 10)
110  4.10.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
2HCL(  5)+                   =1HCL(  4)+1HCL(  6)
110  5. 6.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
1HCL(  5)+1HCL(  6)          =1HCL(  4)+1HCL(  7)
110  5. 7.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
1HCL(  5)+1HCL(  7)          =1HCL(  4)+1HCL(  8)
110  5. 8.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
1HCL(  5)+1HCL(  8)          =1HCL(  4)+1HCL(  9)
110  5. 9.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
1HCL(  5)+1HCL(  9)          =1HCL(  4)+1HCL( 10)
110  5.10.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
2HCL(  6)+                   =1HCL(  5)+1HCL(  7)
110  6. 7.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
1HCL(  6)+1HCL(  7)          =1HCL(  5)+1HCL(  8)
110  6. 8.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
1HCL(  6)+1HCL(  8)          =1HCL(  5)+1HCL(  9)
110  6. 9.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
1HCL(  6)+1HCL(  9)          =1HCL(  5)+1HCL(  0)
110  6.10.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
2HCL(  7)+                   =1HCL(  6)+1HCL(  8)
110  7. 8.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
1HCL(  7)+1HCL(  8)          =1HCL(  6)+1HCL(  9)
110  7. 9.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
1HCL(  7)+1HCL(  9)          =1HCL(  6)+1HCL( 10)
110  7.10.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
2HCL(  8)+                   =1HCL(  7)+1HCL(  9)
110  8. 9.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
1HCL(  8)+1HCL(  9)          =1HCL(  7)+1HCL( 10)
110  8.10.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
2HCL(  9)+                   =1HCL(  8)+1HCL( 10)
110  9.10.                      6.769E-11-4.638E- 3 1.941E-12     0.495     40.246
2H2  (  1)+                  =1H2  (  0)+1H2  (  2)
111  1. 2.                      6.769E-12-4.638E- 3 1.941E-13     0.495     40.246
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1H2 (  1)+1H2 (  2)+          =1H2 (  0)+1H2 (  3)
111  1. 3.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
1H2 (  1)+1H2 (  3)+          =1H2 (  0)+1H2 (  4)
111  1. 4.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
1H2 (  1)+1H2 (  4)+          =1H2 (  0)+1H2 (  5)
111  1. 5.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
1H2 (  1)+1H2 (  5)+          =1H2 (  0)+1H2 (  6)
111  1. 6.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
1H2 (  1)+1H2 (  6)+          =1H2 (  0)+1H2 (  7)
111  1. 7.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
1H2 (  1)+1H2 (  7)+          =1H2 (  0)+1H2 (  8)
111  1. 8.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
2H2 (  2)+                    =1H2 (  1)+1H2 (  3)
111  2. 3.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
1H2 (  2)+1H2 (  3)+          =1H2 (  1)+1H2 (  4)
111  2. 4.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
1H2 (  2)+1H2 (  4)+          =1H2 (  1)+1H2 (  5)
111  2. 5.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
1H2 (  2)+1H2 (  5)+          =1H2 (  1)+1H2 (  6)
111  2. 6.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
1H2 (  2)+1H2 (  6)+          =1H2 (  1)+1H2 (  7)
111  2. 7.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
1H2 (  2)+1H2 (  7)+          =1H2 (  1)+1H2 (  8)
111  2. 8.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
2H2 (  3)+                    =1H2 (  2)+1H2 (  4)
111  3. 4.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
1H2 (  3)+1H2 (  4)+          =1H2 (  2)+1H2 (  5)
111  3. 5.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
1H2 (  3)+1H2 (  5)+          =1H2 (  2)+1H2 (  6)
111  3. 6.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
1H2 (  3)+1H2 (  6)+          =1H2 (  2)+1H2 (  7)
111  3. 7.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
1H2 (  3)+1H2 (  7)+          =1H2 (  2)+1H2 (  8)
111  3. 8.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
2H2 (  4)+                    =1H2 (  3)+1H2 (  5)
111  4. 5.                      6.769E-12-4.638E- 3 1.941E-13     0.495    40.246
```

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1H2 (  4)+1H2 (  5)+          =1H2 (  3)+1H2 (  6)
111  4. 6.                      6.769E-12-4.638E- 3 1.941E-13     0.495     40.246
1H2 (  4)+1H2 (  6)+          =1H2 (  3)+1H2 (  7)
111  4. 7.                      6.769E-12-4.638E- 3 1.941E-13     0.495     40.246
1H2 (  4)+1H2 (  7)+          =1H2 (  3)+1H2 (  8)
111  4. 8.                      6.769E-12-4.638E- 3 1.941E-13     0.495     40.246
2H2 (  5)+                    =1H2 (  4)+1H2 (  6)
111  5. 6.                      6.769E-12-4.638E- 3 1.941E-13     0.495     40.246
1H2 (  5)+1H2 (  6)+          =1H2 (  4)+1H2 (  7)
111  5. 7.                      6.769E-12-4.638E- 3 1.941E-13     0.495     40.246
1H2 (  5)+1H2 (  7)+          =1H2 (  4)+1H2 (  8)
111  5. 8.                      6.769E-12-4.638E- 3 1.941E-13     0.495     40.246
2H2 (  6)+                    =1H2 (  5)+1H2 (  7)
111  6. 7.                      6.769E-12-4.638E- 3 1.941E-13     0.495     40.246
1H2 (  6)+1H2 (  7)+          =1H2 (  5)+1H2 (  8)
111  6. 8.                      6.769E-12-4.638E- 3 1.941E-13     0.495     40.246
2H2 (  7)+                    =1H2 (  6)+1H2 (  8)
111  7. 8.                      6.769E-12-4.638E- 3 1.941E-13     0.495     40.246
   2989.74     52.05    4395.2     117.99
 1.140E-04 9.328E-01 3.999E-02 2.049E-03 1.256E-04 9.204E-06 8.064E-07
 8.447E-08 1.058E-08 1.584E-09 2.215E-02 2.491E-03 3.032E-04 3.992E-05
 5.687E-06 8.767E-07 1.462E-07 2.639E-08 5.153E-09 1.088E-09 2.489E-10
 0.0
     1900.        50.  2.59E-10
     1772.        39.  4.71E-10
     1606.        27.  1.62E-09
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OCHHS,CM160000,MT1.
ACCT(PN=HOPEROC,PBC=7A02006A05,CC=AXXX,OP=A1,JN=OHFR).
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FTN,R=3.
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*D,DATAL.577
1HCL(  9)+1H2 (  6)+          =1HCL( 10)+1H2 (  5)+
*D,DATAL.597
1HCL(  9)+1H2 (  7)+          =1HCL( 10)+1H2 (  6)+
*D,DATAL.617
1HCL(  9)+1H2 (  8)+          =1HCL( 10)+1H2 (  7)+
*D,DATAL.695
1HCL(  6)+1HCL(  9)           =1HCL(  5)+1HCL(  0)
*D,DATAL.705
1HCL(  8)+1HCL(  9)           =1HCL(  7)+1HCL( 10)
*D,DATAL.766,772
 1.140E-04 9.416E-01 3.150E-02 1.764E-03 6.711E-05 1.484E-06 3.134E-08
 1.659E-09 2.555E-10 7.064E-11 2.267E-02 2.106E-03 2.039E-04 1.735E-05
 1.173E-06 6.200E-08 2.625E-09 9.165E-11 2.697E-12 6.757E-14 1.455E-15
 0.0
     236.2 .03215    1.677E-07
     236.2 .03215    2.396E-07
     236.2 .03215    3.422E-07
     236.3 .03216    4.889E-07
     236.3 .03216    6.984E-07
     236.4 .03217    9.978E-07
     236.5 .03218    1.425E-06
     236.6 .03220    2.036E-06
     236.8 .03223    2.456E-06
     237.0 .03226    2.910E-06
     237.2 .03229    3.525E-06
     237.5 .03233    4.385E-06
     237.9 .03238    5.644E-06
     238.3 .03245    6.236E-06
     238.9 .03252    6.991E-06
     239.5 .03260    7.956E-06
     240.2 .03270    9.585E-06
     241.0 .03282    1.102E-05
     242.0 .03296    1.202E-05
     243.2 .03312    1.352E-05
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244.5	.03330	1.574E-05
246.1	.03352	2.082E-05
248.3	.03382	2.490E-05
250.9	.03419	3.556E-05
254.8	.03473	3.974E-05
259.1	.03533	3.339E-05
262.7	.03582	3.005E-05
265.8	.03626	3.236E-05
269.1	.03672	2.928E-05
269.2	.03672	2.929E-05
272.1	.03712	3.200E-05
275.0	.03754	2.978E-05
277.7	.03792	3.291E-05
280.5	.03830	3.608E-05
283.5	.03871	3.260E-05
286.0	.03906	3.657E-05
288.6	.03943	3.453E-05
290.9	.03975	3.991E-05
293.4	.04010	4.262E-05
295.9	.04045	3.719E-05
297.9	.04073	4.182E-05
300.0	.04102	4.707E-05
302.2	.04133	4.178E-05
304.0	.04158	4.542E-05
305.8	.04183	4.855E-05
307.5	.04207	4.422E-05
309.0	.04228	5.062E-05
310.6	.04250	5.739E-05
312.1	.04272	6.176E-05
313.6	.04293	6.343E-05

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